Design Optimization of Waveguide Bends in Photonic Crystals

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In this paper, a fast and robust optimization scheme is presented and applied to the optimal design of planar photonic crystals. It is based on a parallel hybrid (stochastic-deterministic) algorithm coupled to a semi-analytic solution of "full Maxwell" equations by multiple scattering technique. The numerical results of the optimal design of different waveguide bends are presented.

***Index Terms*—Hybrid algorithms, multiple scattering technique (MST), photonic crystals.**

I. Introduction

CONVENTIONAL planar waveguides confine light by total internal reflection. One of the weaknesses of such waveguides, however, is that creating bends is difficult. Indeed, as soon as the radius of the bend becomes comparable with the wavelength, much of the light is lost [1]. This is a serious drawback if one looks for realization of optical "integrated circuits," as the space required for large-radius bends is often unavailable.

Mainly due to this reason, photonic crystals [2]–[7] have received increasing interest in recent years. Indeed, photonic crystal may guide light by means of a different physical mechanism with respect to the total internal reflection. To illustrate it in a simple way, let us consider a 2-D photonic crystal, i.e., a structure whose dielectric constant is independent of one of the directions of space, while showing a periodic pattern with respect to the two remaining ones. A proper choice of the dielectric materials, and of the shape of the periodic pattern may permit to obtain a *band-gap*: an electromagnetic wave having frequency within the gap is not allowed to travel through the crystal, whatever its propagation direction is.

Suppose now that a linear defect is created in such a crystal, and that a light beam with frequency within the gap is injected into it. Light is confined in the vicinity of the defect simply because, due to the band-gap, it may not spread through the crystal. [8]–[10]. This occurs even if the linear defect does not follow a straight path, but it rather bends, even at sharp angles. This way, realization of a really compact integrated optical circuit becomes possible [11]–[13].

So far, several proposals have been formulated, both theoretically and experimentally, to show that guiding through sharp bends or junctions may be obtained indeed. However, as it occurs in any high-frequency circuit, either at microwaves or in optics, abrupt deviations of the light path from the straight one may cause mode-mixing problems at intersections. If not properly engineered, this might cause large reflections and poor transmissions through the bends.

A way to circumvent this problem is that of modifying the crystal structure in the vicinity of the bends. Indeed, the physics of processes which takes place in the vicinity of abrupt deviations from the straight light path may be simply described as follows. The field in a straight waveguide may always be expressed as a sum of orthogonal modes. When the waveguide shape is varied, new set of modes are created. The mode which was propagating in the straight waveguide projects onto this new set of modes and couples to several of them. Usually, only one of the modes is allowed to propagate, while the remaining ones are under cut-off. This, in turn, means that the wave impedance of the new modes is real for one of them, and imaginary for the rest. The ensemble of the straight waveguide and the bend (and anything else which is beyond the bend) may then be represented as an equivalent transmission line closed on a load which exhibits both a real part (which is responsible for the propagation of the light trough the bend) and an imaginary one, due to the local excitation of higher order modes. The problem of increasing the transmission through the bend is then equivalent to the problem of matching a load: the imaginary part of the load needs to be cancelled, or at least, reduced. At microwaves, specifically in the framework of propagation within metallic waveguides, this is customarily done by introducing *ad-hoc* designed posts in the vicinity of the waveguide shape deviation. In the framework of photonic crystal waveguides, a similar technique may be used: The geometry of the crystal surrounding the bend needs to be properly modified.

Unfortunately, an analytical way to predict the arrangement of the atoms (irrespectively air holes in dielectrics, or dielectric pillars is air) which gives the best transmission can not be found. The optimization process must be done via extensive numerical simulations. To this end, a numerical code having the following properties needs to be used.

- The code must be able to account for full-vector fields in the presence of large index discontinuities.
- In addition, it must include an optimization routine able to rapidly converge to a stable solution.

As for the field computation, several different techniques have been proposed and tested in the framework of photonic crystals. Many of those, like the finite-difference time-domain (FDTD) technique [14], the cell's method [15], the Green's tensor approach [16], the Fourier-modal method [17] or the eigenmode-expansion method [18], [19] share a common concept, that sets similar pros and cons. As a matter of fact, in those techniques the starting point is *discretization* of the computational domain, or of a part of it. This makes the codes very broad-scope: in fact, since any object may be discretized, the numerical techniques may operate with any kind and shape of dielectrics in the photonic crystal. The price to pay for this wide generality is the high computational effort, both in terms of memory allocation and computational time. Indeed, the code

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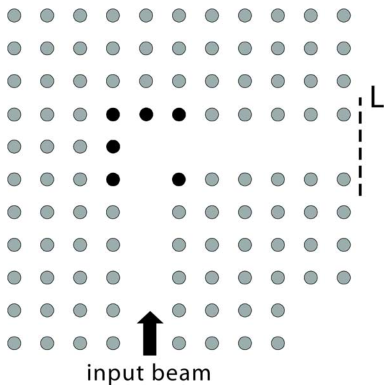

Fig. 1. Square array of infinitely long dielectric pillars (refractive index $n = 3.4$, radius to pitch ratio $r/a = 0.2$) embedded in air, with a sharp 90° bend obtained by removing a line of pillars from the square lattice. The optimization variables are the positions and radii of the black circles.

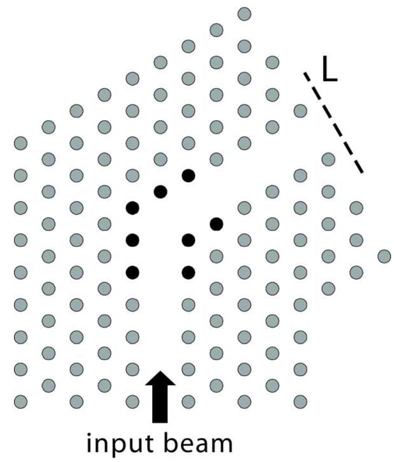

Fig. 2. Triangular array of infinitely long dielectric pillars (refractive index $n = 3.4$, radius to pitch ratio $r/a = 0.2$) embedded in air, with a sharp 60° bend obtained by removing a line of pillars from the triangular lattice. The optimization variables are the positions and radii of the black circles.

accuracy improves with the number of samples that are used to discretize the objects in the photonic crystal.

However, since we aim at coupling the numerical field computation to an optimization routine, which, in turn, means that the field will need to be re-computed several times before the optimal solution is found, we developed an *ad hoc*, fast and robust, procedure. It is based on hybrid algorithms coupled to a semi-analytic solution of "full Maxwell" equations by multiple-scattering technique (MST) [20], that does not allow to handle generic geometries as the codes above, but converges rapidly to the solution. The proposed approach is applied to the study of light transmission through 60°–90°–120° bends in planar photonic crystals. Indeed, any real structure would be realized with finite-thickness rods etched in slab geometry, and 2-D calculations would certainly be not accurate enough for such structures. However, we note that as a three-dimensional version of the MST technique is available [21], the optimization routine may be easily extended to real-world 3-D cases too.

II. Problem Description

As a test geometry, first we considered the case of a square array of infinitely long dielectric pillars (refractive index $n_d = 3.4$ and radius to pitch ratio $r/a = 0.2$) embedded in air, with a sharp 90° bend obtained by removing a line of pillars from the square lattice (Fig. 1).

In the optimization problem, the objective function is given by the flux of the Poynting vector through line L. As design variables, the radii and/or the positions of some pillars (e.g., black circles, in Fig. 1) around the bend have been chosen.

Thereafter, we focused on a triangular array of infinitely long dielectric pillars (refractive index $n_d = 3.4$ and radius to pitch ratio $r/a = 0.2$) embedded in air. In this framework, two different cases have been studied: a sharp 60° bend (Fig. 2) and a sharp 120° bend (Fig. 3), both obtained by removing a line of pillars from the triangular lattice.

The objective function is given by the flux of the Poynting vector through line L of Figs. 2–3, respectively. As design variables, the radii and/or the positions of some pillars (black circles) around the 60° (Fig. 2) and 120° (Fig. 3) bends have been chosen.

The square lattice exhibits a band gap only for the TM polarization (i.e., with the electric field parallel to the pillars) in the

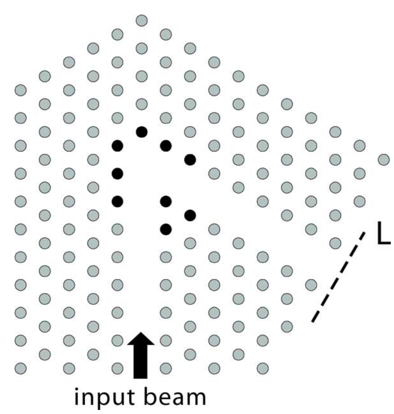

Fig. 3. On the left side: Triangular array of infinitely long dielectric pillars (refractive index $n = 3.4$, radius to pitch ratio $r/a = 0.2$) embedded in air, with a sharp 120° bend obtained by removing a line of pillars from the triangular lattice. The optimization variables are the positions and radii of the black circles.

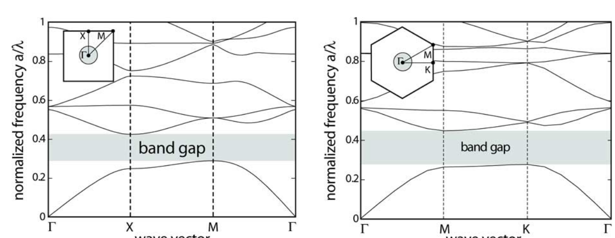

Fig. 4. On the left side: TM band structure for the square array of infinitely long dielectric pillars. On the right side: TM band structure for the triangular array of infinitely long dielectric pillars.

frequency range $0.288 < a/\lambda < 0.423$ (Fig. 4-left); the triangular lattice exhibits a band gap for the TM polarization in the frequency range $0.275 < a/\lambda < 0.446$ (Fig. 4-right).

In the numerical simulations, a normalized frequency $a/\lambda = 0.35$ for the TM polarization has been used.

A. Optimization Procedure

The optimization procedure is based on a hybrid approach which combines a parallel genetic algorithm (GA), for global minimum search [23] and a deterministic algorithm (DA), for local refinement [24], coupled to a semi analytic solution of "full Maxwell" equations by multiple scattering technique (MST).

The MST exploits the following idea: photonic crystals are usually realized by etching circular holes in an high-index dieletric, or by arranging pillars with circular cross-section in a low-index substrate. One may recognize that both the holes and the pillars are geometrically "simple" objects, so that one may look for *rigorous solutions* of the Maxwell's equations in analytical form. The basic idea is the following. If we want to describe the field inside or around a cylindrical object, the best choice we have is to write the field as a sum of the "natural" modes of cylindrical objects, the *cylindrical harmonics*. With this choice, we do not need to make any discretization, and we may reasonably expect that a few terms will be enough to properly approximate the field. This, in turn, means that the time needed for the field computation may be reasonably small.

The final optimal design is achieved by means of an iterative scheme. Each point in the search space represents a different design, to be submitted from the search algorithm $(\mathrm{GA}+\mathrm{DA})$ to the MST analysis tool. Then the MST return the relevant parameters (fitness measure) to the search algorithm until a stop condition is reached.

The GA is intrinsically parallel, and thus it has been efficiently compiled for execution on a parallel hardware using the OpenMP library.

The design variables are coded in strings using a Gray standard format and the operators, except minor details, are the classical ones proposed by Holland [22] and revised by Goldberg [23]. In particular, a roulette-wheel *selection* is adopted, based on string fitness values: the higher the fitness value of strings (individuals), the higher the probability of their copies in next generation; then, if $\{k_1\}$ are strings assigned at least one copy, $\{k_2\}$ are strings assigned at least two copies and so on, the new generation is created arranging first the $\{k_N\}$ strings, then $\{k_{N-1}\}$ strings and so on until the new population is completed. This arrangement is expected to favour the recombination between low performance elements by *crossover* and preserve strings with best fitness values. As for *mutation*, a uniform probability distribution over each string is imposed.

Neither coupling restrictions nor "niche techniques" were applied, but an exponential fitness scaling mechanism is implemented. If $f(\mathbf{x})$ is the objective function, with $\mathbf{x}$ the design variable array, then the fitness function should be

$$f_f(\mathbf{x}) = e^{\alpha f(\mathbf{x})} \tag{1}$$

being α a damping coefficient which can vary through generations, controlling the selective effect of the exponential function.

An efficient DA, based on a well-established package for constrained optimization developed by Powell [24], is used for local minimum refinement.

B. Numerical Results

Several numerical analyses have been carried out varying either the position or the dimension of the selected pillars, or both. The upper and lower bounds for the design variables have been chosen so to avoid overlap of the pillars; the values used in the simulations are reported in Tables I and II, for test case 1 (rectangular array) and test cases 2–3 (triangular arrays), respectively.

TABLE I
DESIGN VARIABLES—UPPER AND LOWER BOUNDS FOR TEST CASE 1

	x and y coordinate	radius
position	$\pm$ 0.29	-
radii	-	0.01 $\div$ 0.49
position & radii	$\pm$ 0.22	0.01 $\div$ 0.27

TABLE II
DESIGN VARIABLES—UPPER AND LOWER BOUNDS FOR TEST CASES 2-3

	x coordinate	y coordinate	radius
position	$\pm$ 0.22	$\pm$ 0.29	-
radii	-	-	0.01 $\div$ 0.42
position & radii	$\pm$ 0.20	$\pm$ 0.23	0.01 $\div$ 0.22

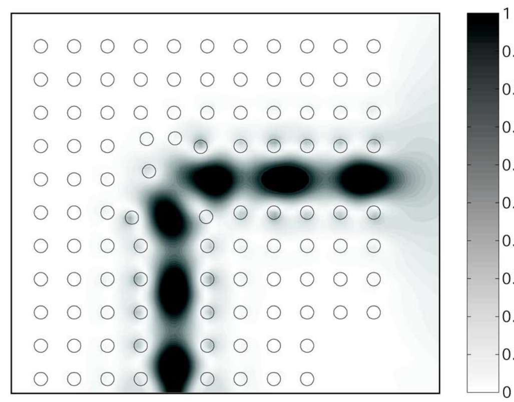

Fig. 5. Optimal design of a 90° bend by moving only cylinders positions: normalized modulus of the electric field.

The overall time of the optimization procedure is problem dependant and relies mainly on the number of pillars, cylindrical harmonics, design variables, elements (individuals) of each population, iterations. In the MST code, the field scattered by each pillar has been expanded into seven cylindrical harmonics. The structures we considered contained 116, 104, and 141 cylinders for the 60°, 90°, and 120° bends cases, respectively, so that the overall number of unknowns to be determined by the MST was 812, 728, and 987, respectively. The memory required to store this amount of unknowns was in the order of 50 MB for four threads simultaneously. The code, developed in Fortran 90, took approximately 10 seconds to perform the calculation of the scattered field on a double Dual-Core Intel® Xeon™ 3.2-MHz workstation with 8GB RAM.

Figs. 5–7 show the optimized results we have obtained in the three cases listed above. The figures represent a top view of the modulus of the electric filed along the waveguides. Along with the field, the arrangement of dielectric pillars is shown. Some of them are off-centered with respect to the regular lattice: this is the result of the optimization routine, which has moved them in order to increase the transmission. The population of pillars that has been considered for the optimization in each of the three cases is shown in Figs. 1–3, where they appear as black filled circles. It may be observed that they seed in the vicinity of the bend, and most remarkably, only in the first row of pillars which directly borders the waveguide core. This is due to the fact that the electric field is tightly confined in the waveguide core. Indeed, owing the band-gap properties of the lattice, the amplitude of the field dramatically drops if it tries to propagate through the lattice itself. This, in turn, means that only very

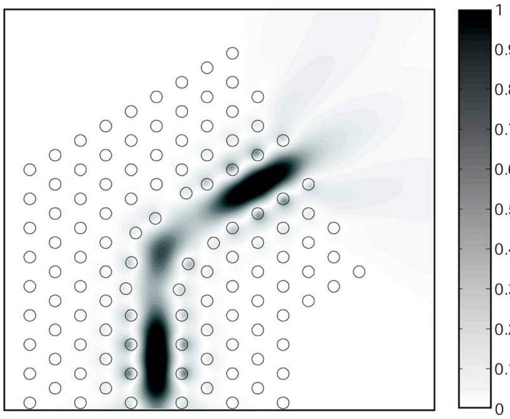

Fig. 6. Optimal design of a 60° bend by moving only cylinders positions: normalized modulus of the electric field.

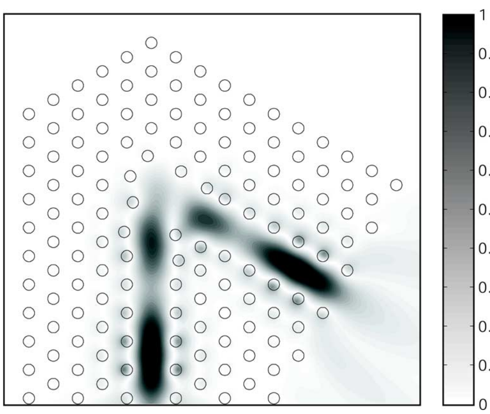

Fig. 7. Optimal design of a 120° bend by moving only cylinders positions: normalized modulus of the electric field.

TABLE III
TRANSMISSION IMPROVEMENT

optimization variables \ bend angle	90°	60°	120°
position	28%	150%	385%
radii	28%	150%	388%
position & radii	28%	150%	388%

small tails of the field may experience changes of the pillars beyond the first row. In other words, if one of such pillars is modified, its impact on the overall field propagation is almost negligible.

Table III shows the percentage increase of the power flux as integrated along the lines marked with letter "L" in Figs. 1–3, that we obtained with the optimized structures in each of the three cases we considered. As it may be seen, the change of pillars' position or dimensions (or both) leads almost always to the same improvement factor. A slight difference is observed only in the case of the 120° bend: in this case, modification of the pillars' radii allows for a minor further improvement to be obtained with respect to the case of modification of pillars' positions. Anyway, in each optimal design the output power exceeds the 90% of the incident power.

III. CONCLUSION

A fast optimization routine has been developed for the study of wave propagation in planar 2-D photonic crystals. The routine couples a rigorous full-vector numerical solution of Maxwell's equations, which is able to handle problems comprising an arbitrary number of pillars or holes embedded in a homogeneous dielectric substrate, to an hybrid algorithm which bases on a genetic approach for global minimum search of a given objective function and a deterministic procedure for local refinement. The routine has been applied to the problem of maximizing the transmission through sharp bends in photonic crystal.

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