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Systematic design of photonic crystal structures using topology optimization: Low-loss waveguide bends

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Topology optimization is a promising method for systematic design of optical devices. As an example, we demonstrate how the method can be used to design a 90° bend in a two-dimensional photonic crystal waveguide with a transmission loss of less than 0.3% in almost the entire frequency range of the guided mode. The method can directly be applied to the design of other optical devices, e.g., multiplexers and wave splitters, with optimized performance. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1688450]

A range of perspectives exist for using photonic crystal (PC) based waveguides in optical components. This has led to a considerable research interest in the design of waveguide bends with low transmission loss.

PCs can be created by periodic arrangements of materials with different dielectric properties such as, e.g., dielectric columns in air or holes in a dielectric base material.[1] Such two-dimensional periodic configurations may forbid the propagation of plane polarized light in specific frequency ranges, i.e., the so-called photonic band gaps (PBGs). A waveguide can be created by removing one or several lines of columns or holes resulting in defects that support guided modes in the PC structure.[2]

A key advantage of PC waveguides is that bends can be created with very little or no transmission loss even with bend curvatures as small as the wavelength. Although PC waveguides generally offer low losses compared to traditional dielectric waveguides, much effort has been devoted to reducing these losses to a minimum over larger frequency ranges. Waveguides with dielectric columns in a rectangular configuration have been subjected to extensive computations[3] and recently waveguides with holes etched in a triangular pattern in a dielectric have been analyzed thoroughly both theoretically and experimentally.[4]

Despite the considerable amount of studies on PC waveguides that have appeared, few papers have dealt with optimization or the inverse problem of obtaining structures with optimal or desired properties. The few papers that have appeared (e.g., Refs. 5 and 6) have considered simple geometry variations like existence/nonexistence of holes or rods or variations of hole or rod diameters. The topology optimization method[7,8] is a gradient-based optimization method that creates optimized designs with no restrictions on resulting topologies and can thus be used to create designs with previously unattainable properties. The topology optimization method has in the last decade been used to design materials with extremal properties, compliant and multiphysics mechanisms, piezoelectric actuators, and plenty more.[8] Here, the transmission loss in a column-based waveguide with a 90° bend is systematically minimized by the topology optimization method. This work applies a gradient-based method to waveguide optimization, thus creating optimized waveguides with much less computational effort and more design freedom than previously used genetic or other heuristic algorithms.

The analyses and optimization presented here are based on a time-harmonic two-dimensional finite element (FE) model. Unwanted reflections from the input and output waveguide ports are eliminated by using anisotropic perfectly matching layers (PML) with the waveguide structure continued into the damping layers. This ensures that reflections from the input and output ports are kept to a minimum.[9] The loss in the waveguide bend is found by comparing the transmission of energy through the bend waveguide to that of a straight waveguide.

The computational model is shown in Fig. 1 and consists of the actual computational domain and two additional PML areas. For this example we consider propagation of an E-polarized wave governed by

$$\nabla^2 E + \omega^2 \left(\frac{n}{c}\right)^2 E = 0, \tag{1}$$

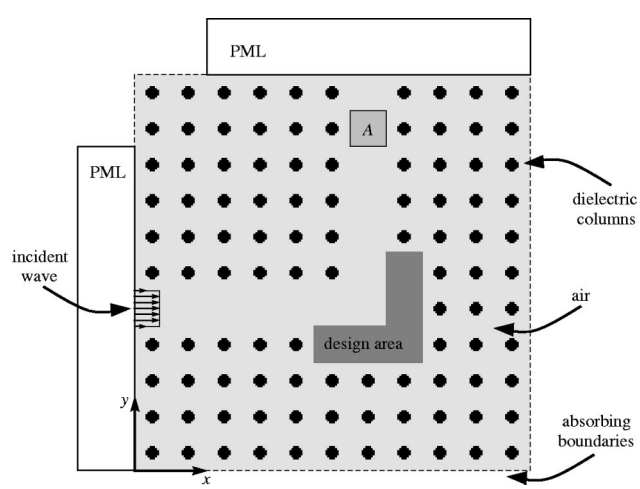

FIG. 1. Waveguide with a 90° bend line defect in a periodic configuration of dielectric columns ($n=3.4$) in air. Unwanted reflections from the input and output waveguide ports are eliminated by using anisotropic PML regions, and the energy transmission through the waveguide is evaluated in the unit cell denoted A.

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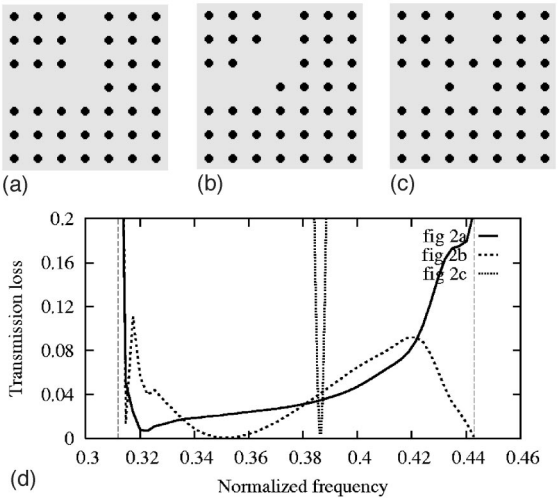

FIG. 2. (a), (b), and (c) Three standard corner designs, and (d) the corresponding transmission losses vs normalized frequency $\omega a/(2\pi c)$ computed in the guided mode frequency range (indicated by vertical dashed lines).

where ω is the wave frequency, $n=n(x,y)$ is the refractive index, c the speed of light, and $E=E(x,y)$ is the electric field. In the PML regions the governing equation is modified to obtain anisotropic damping properties.[9]

An incident wave is specified by the boundary condition: $\mathbf{n}\cdot\nabla E=2i\omega(n/c)$, and on the other boundaries of the computational domain the condition: $\mathbf{n}\cdot\nabla E+i\omega(n/c)E=0$, ensures normal absorbing boundaries. The vector $\mathbf{n}$ is in both cases an outward pointing normal vector.

We use a FE discretization of Eq. (1) (as well as the PML equation and the boundary conditions) with $\approx 115\,000$ rectangular bilinear elements. This leads to a set of linear complex equations:

$$\mathbf{S}(\omega)\mathbf{u}=\mathbf{f}(\omega), \tag{2}$$

where $\mathbf{S}(\omega)$ is a frequency-dependent system matrix, $\mathbf{f}(\omega)$ a frequency-dependent load vector, and Eq. (2) is solved for the vector $\mathbf{u}$ containing the discretized nodal values of the field E.

The energy transmission through the waveguide is found by computing the time-averaged Poynting vector through the area A (Fig. 1):

$$\mathbf{p}=\{p_x p_y\}^T=\frac{\omega}{2a}\int_A \Re(i(\nabla E)E^*)dA, \tag{3}$$

where a is the lattice constant and E^* is the complex conjugate field.

We consider a square configuration of unit cells with centered dielectric columns ($n=3.4$) with a diameter of $d=0.36a$ placed in air. This configuration has been shown to have a PBG for E-polarized waves for $\omega=0.302-0.443(2\pi c/a)$.[3] Each unit cell is discretized using 19×19 finite elements which is adequate to reproduce this band gap frequency range. The waveguide model (Fig. 1) consists of 11×11 unit cells with 2 PML regions attached (each having a depth of 11 unit cells). By removing a line of columns a waveguide is created that supports a single guided mode in the frequency range $\omega=0.312-0.443(2\pi c/a)$.[3]

First we consider three standard corner designs [Figs. 2(a)–2(c)] and compute their corresponding transmission loss [Fig. 2(d)]. The zero-curvature bend [Fig. 2(a)] displays a loss up to $\approx 20\%$ in the guided mode frequency range. By repositioning a single column [Fig. 2(b)] the loss is reduced and full transmission through the bend is reached for $\omega\approx 0.352(2\pi c/a)$. In Fig. 2(c) the corner is designed with two extra columns in the path and via resonant tunneling nearly full transmission is obtained for $\omega\approx 0.386(2\pi c/a)$, but the loss increases significantly for other frequencies. The losses computed with our FE model have been verified against results previously obtained by using different computational methods, e.g., FDTD simulations.[3,10]

In order to reduce the bend loss we now apply the topology optimization method to design the corner geometry. We choose a design area in the corner region consisting of five unit cells (Fig. 1) and designate a single design variable x_i to each corresponding finite element in the region:

$$x_i\in\mathbb{R}|0\leqslant x_i\leqslant 1 \quad \text{for } i=1,N, \tag{4}$$

that is, in total N design variables where in this case $N=5\times 19^2=1805$. We use a linear interpolation scheme for the dielectric property $\varepsilon=n^2$ of the material in the design region elements:

$$n_i^2=n_1^2+x_i(n_2^2-n_1^2), \tag{5}$$

where $n_1=1$ and $n_2=3.4$ corresponding to air and the dielectric, respectively. That is, for $x_i=0$ the element will take the property of air, for $x_i=1$ the property of the dielectric, and for any intermediate value of x_i we have some intermediate dielectric property. As will appear in the following, these intermediate values practically vanish in the optimized design which may be explained by the fact that a high index contrast is favorable for creating wide band gaps.

In this example we choose as our optimization goal to *maximize* the y component of the time-averaged Poynting vector p_y in the cell A for a number M of target frequencies $\overline{\omega}_j$, $j=1,M$. Our optimization objective can thus be formulated as

$$\begin{aligned} &\max_{x_i} \quad C=\sum_{j=1}^{M} p_y(\mathbf{u}_j) \\ &\text{subject to:} \quad \mathbf{S}(\overline{\omega}_j)\mathbf{u}_j=\mathbf{f}(\overline{\omega}_j), \quad j=1,M, \\ &\qquad\qquad 0\leqslant x_i\leqslant 1, \qquad i=1,N. \end{aligned} \tag{6}$$

The optimization problem in Eq. (6) is solved using an iterative procedure (see Ref. 8 for details). Given an initial material distribution x_i [here chosen as the structure in Fig. 2(a)] the objective C is computed along with the sensitivities with respect to the design variables. Using the mathematical programming tool MMA[11] this is transformed into an improved design suggestion, i.e., updated values of x_i, and C is again computed. This procedure is repeated until the design x_i no longer changes significantly between successive iterations. The sensitivities are found analytically using the adjoint method,[8,12] which is computationally very cheap since it only requires solving the system equation (2) for one additional load case. Although we here use a simple objective function it should be emphasized that any numerically quantifiable objective function can be used, and since we are us-

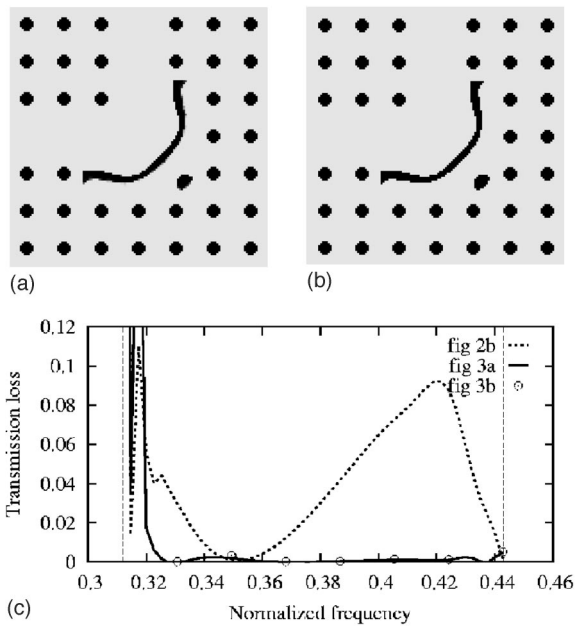

FIG. 3. (a) Optimized corner design, (b) postprocessed design with black and white elements only, and (c) transmission losses for the two designs and for a standard corner design.

ing a mathematical programming solver (MMA) extra geometric or behavioral constraints can easily be added to Eq. (6).

In our example we maximize the output energy for three frequencies $\overline{\omega}=0.34,0.38,0.42(2\pi c/a)$ in order to minimize the loss in a large frequency range. Figure 3(a) shows the optimized design obtained after about 500 iterations of the optimization algorithm (about 20 s per iteration on a 2.66 GHz computer). It is evident that the optimized design is practically ''black–white,'' i.e., almost free of elements with intermediate x_i values between 0 and 1. In Fig. 3(b) is shown a postprocessed design where the few intermediate values that do appear are forced to either 0 or 1 with a simple filter. Figure 3(c) shows the transmission loss for the optimized and for the postprocessed designs. Noticeable is that a loss below 0.3% is obtained in the entire frequency range from $\omega\approx 0.325$ to $0.440(2\pi c/a)$.

Although low transmission loss is obtained using a two-dimensional model, the question of out-of-plane losses for the optimized waveguide remains open and should be addressed using a three-dimensional (3D) model (the optimization algorithm can immediately be used with a 3D model). However, the method is naturally also applicable to the design of waveguides based on holes in a dielectric and these are generally known to be less prone to out-of-plane losses. In addition to waveguide bends the method can be applied to systematic design of a large variety of optical devices such as, e.g., wave-splitters, multiplexers, and other more complex objectives. Future work will address these issues and we are also expecting to test optimized devices experimentally in the near future. Previous work by the authors has considered design of similar devices for elastic waves.[12]

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