Optimization of photonic crystal cavities

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***Abstract*— We present optimization of photonic crystal cavities. The optimization problem is formulated to maximize the Purcell factor of a photonic crystal cavity. Both topology optimization and air-hole-based shape optimization are utilized for the design process. Numerical results demonstrate that the Purcell factor of the photonic crystal cavity can be significantly improved through optimization.**

Keywords—Photonic crystal; cavity; topology optimization; shape optimization

I. Introduction

Photonic crystal cavities (PhCCs) have unique properties by confining light in a wavelength-size volume with very small loss. PhCCs exhibit high quality factor (Q) and small mode volume (V). This makes PhCCs promising building blocks for future integrated photonic circuits [1].

Previously, several studies were presented to design PhCCs to increase the Q factor while decreasing the modal volume (V), i.e. to enhance the Purcell factor (F_p), which is proportional to Q/V. Most of the studies focused on shape optimization of PhCCs using geometrical perturbations, where the Purcell factor was enhanced by trial-and-error approaches through extensive simulations by changing locations or radii of air holes [2].

More recently, an optimization formulation was presented to optimize the Purcell factor of PhCCs by maximizing the frequency-averaged local density of state (LDOS) [3], where topology optimization was employed to design PhCCs. However, PhCCs presented in the paper are hardly manufacturable due to lack of imposed length scale.

In this study, we employ the optimization formulation presented in Ref [3] to design PhCCs with high Purcell factor. Both topology optimization and air-hole based shape optimization are utilized to design PhCCs. In the topology optimization approach, a robust formulation is utilized to ensure the manufacturability of the designed PhCCs. In the shape optimization, the PhCCs are parameterized using a set of masks. Each mask consists of a circle to represent one air hole in PhC. PhCCs with high Purcell factor are designed by optimizing the locations of circles in the selected masks.

II. Otpimization problem

In this paper, we study a frequency-domain Maxwell problem, governed by:

$$\nabla \times \nabla \boldsymbol{E}(\boldsymbol{x}) - \varepsilon(\boldsymbol{x})\omega^2 \boldsymbol{E}(\boldsymbol{x}) = i\omega \boldsymbol{J}(\boldsymbol{x}) \tag{1}$$

The structure is discretized with a regular mesh. Eq. (1) is solved numerically using the finite element methods.

The Purcell factor is an approximation of a more fundamental quantity, i.e. the local density of state (LDOS) which is defined as the density of state per unit frequency per unit volume. For a specific polarization, LDOS is denoted by $LDOS(\omega, \boldsymbol{x}')$, which represents the LDOS for a polarization in direction j. It is proportional to the power radiated by a dipole in direction j at the position $\boldsymbol{x}'$ with a frequency ω,

$$LDOS(\omega, \boldsymbol{x}') = \frac{12}{\pi} P(\omega, \boldsymbol{x}')_j = -\frac{6}{\pi} \mathrm{Re}\left[\int \boldsymbol{J}'(\boldsymbol{x}) \cdot \boldsymbol{E}(\boldsymbol{x})\, d\boldsymbol{x}\right] \tag{2}$$

where $\boldsymbol{J}'(\boldsymbol{x})$ denotes conjugate of $\boldsymbol{J}(\boldsymbol{x})$.

The optimization formulation for enhancing Purcell factor can be formulated to maximize the frequency-averaged LDOS, stated as [3]:

$$\max_{\varphi} \int_{-\infty}^{-\infty} LDOS(\omega, \boldsymbol{x}')\, w(\omega) d\omega \tag{3}$$

where $w(\omega)$ is the weight function, here we choose the square of a Lorentzian weight function. The detailed calculation of the objective in Eq. (3) can be found in Ref [3].

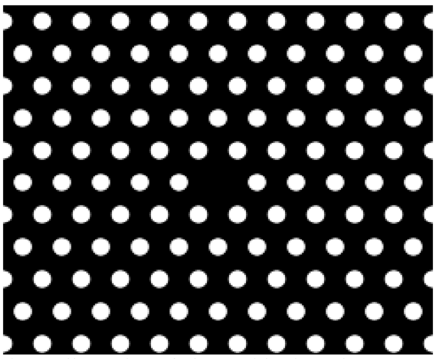

Fig. 1. Illustration of PhCC with triangular patterned air holes.

The PhCC consisting of triangular patterned air holes shown in Fig. 1 can be described using a set of masks. Each mask consists of a circle, the region inside the circle is assigned to be air and the region outside the circle is assigned to be Si. The physical density for element e resulting from a mask can be calculated as:

$$\rho_e = H(\boldsymbol{x}_e, \boldsymbol{y}_i, r_i) = 1/\left(1 + \exp\left(-\beta\left(\frac{\|x_e - y_i\|^2}{r_i^2} - 1\right)\right)\right) \tag{4}$$

here $\boldsymbol{x}_e$ is the centroid of element e, $\boldsymbol{y}_i$ and r_i are the location and radius of the ith mask, respectively, and β is a

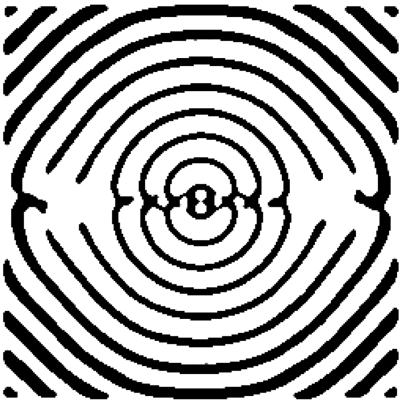

Fig. 2. Optimized Hz-polarized PhCC using topology optimization for given frequency $\omega_0 = 0.32 * 2\pi/a$.

regularization parameter. The final physical density of element e resulting from all M mask is

$$\bar{\rho}_e = \prod_{i=1}^{M} H(\boldsymbol{x}_{e,}\boldsymbol{y}_i, r_i) \qquad (5)$$

In robust topology optimization [4], the physical density $\bar{\rho}_e$ is projected from the element-wise design variables ρ_e using a threshold projection. The manufacturability of the design can be ensured by considering several design realizations through choosing different thresholds. More details can be found in Ref [4].

The element material property can be described by the physical density $\bar{\rho}_e$ as:

$$\varepsilon_e = \bar{\rho}_e(\varepsilon_2 - \varepsilon_1) + \varepsilon_1 \qquad (6)$$

where ε_e is the relative permittivity of element e, ε_1 is relative permittivity of air and ε_2 is the relative permittivity of Si.

The sensitivities of the objective with respect to design variables can be calculated using adjoint sensitivity analysis, which is not presented here [5]. The optimization problem is solved by the globally convergent version of the method of moving asymptotes (GCMMA) from Svanberg [6].

III. Results

In this paper, we focus on designing 2D PhCCs for Hz-polarized mode. The direction of the dipole source is along the horizontal direction.

In the case of topology optimization, we aim at designing a PhCC at the center frequency of $\omega_0 = 0.32 * 2\pi/a$. Fig. 2 presents the optimized PhCC with initial guess as air. Compared with the design presented in Ref [3], length scale has been demonstrated by the presented design without element-wise feature, which guarantees the manufacturability of the design. The length scale of the optimized design is imposed by considering three different design realizations. However, the enhancement of manufacturability is obtained at the cost of the Purcell factor. The optimized design shows lower Purcell factor compared to the one in Ref [3].

In the second example, we aim at designing air-hole-based PhCC with parameterization presented in Eqs (4)–(5). The initial design is chosen as the L1 cavity with one air hole missing at the center of the photonic crystal as shown in Fig. 1. In this case, we choose the design variables as locations of air holes of the first three rows closest to the center of the cavity. The optimized design is presented in Fig. 3. Compared to the initial guess, the objective has been increased significantly,

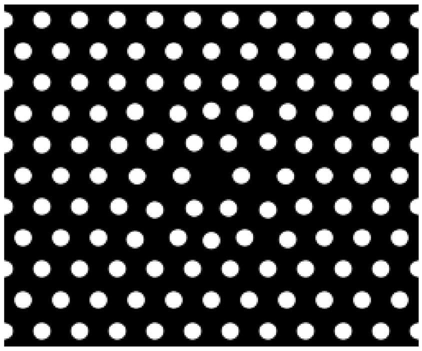

Fig. 3. Optimized Hz-polarized PhCC using shape optimization for given frequency $\omega_0 = 0.2249 * 2\pi/a$.

which indicates that the Purcell factor has been increased significantly.

In this paper, we focused on designing 2D PhCCs using topology optimization and shape optimization by solving a scattering problem. The optimization can be applied directly for 3D PhCC design. Optimized 3D PhCCs will be presented at the conference.

Acknowledgments

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