Two-stage design method for realization of photonic bandgap structures with desired symmetries by interference lithography

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Abstract: Interference lithography for the fabrication of photonic crystals is considered. A two-stage design method for realization of photonic bandgap structures with desired symmetries is developed. An optimal photonic crystal with a large bandgap is searched by adjusting some parameters while keeping some basic symmetry of the unit cell unchanged. A nonlinear programming method is then used to find the optimal electric field vectors of the laser beams and realize the desired interference pattern. The present method is useful for a rational and systematical design of new photonic bandgap structures.

OCIS codes: (260.3160) Interference; (220.3740) Lithography; (220.4000) Microstructure fabrication; (000.3860) Mathematical methods in physics

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1. Introduction

A photonic crystal is an artificial structure which has a periodic modulation of dielectric constant on a length scale of wavelength (see e.g. [1–3]). Several techniques have been developed for the fabrication of photonic crystals in optical regime [4–9]. Compared with the e-beam lithography [4] and self assembly techniques [5], the interference lithography [6–9] is a relatively simple and inexpensive way to generate periodic structures over large areas with high resolution. The simplest example of the interference lithography is to produce a sinusoidal intensity pattern in space by combining two coherent wave fronts. By exposing a layer of photoresist to this interference pattern, a one-dimensional grating can be formed. By combining more than two beams, two-dimensional (2D) and even three-dimensional (3D) periodic structures can be formed. Fabrication of photonic crystals with the interference lithography was first proposed and implemented in [6], where a 2D triangular pattern in a layer of photoresist was fabricated and then served as an etching mask to etch a high index substrate. This approach was extended to create 3D photoresist structures in [7].

The symmetry of the pattern (or motif) within the unit cell of a photonic crystal is often important and photonic crystals with some symmetry are desirable in many applications [10–12]. The symmetry of the interference pattern is determined by the configuration of the laser beams, i.e., the number of the laser beams, the wave-vectors, the phases, the polarization states and the power ratios of these beams. The wave-vectors of the laser beams determine the translational symmetry and the lattice constant. The effects of the relative phases of the beams were discussed in [13]. The polarization effects were considered in [14], where the maximal contrast of the interference pattern was searched, however, regardless of the symmetry of the unit cell (and thus the symmetry of the resultant photonic crystal can not be predicted). In the present paper, we introduce a two-stage design method for realization of photonic bandgap structures with desired symmetries. First we search an optimal photonic crystal with a large bandgap by adjusting some parameters while keeping some basic symmetry of the unit cell unchanged. Then we use a nonlinear programming method to find the optimal electric field vectors of the laser beams which give the desired interference pattern with a maximal contrast.

2. The two-stage design method

2.1. *Stage 1: Optimization of photonic bandgap structures with desired symmetries*

The distribution of the light intensity created by the interference of N coherent beams can be written as

$$I(\overrightarrow{r}) = \sum_{l,m=1}^{N} \overrightarrow{E_l}(\overrightarrow{r}) \cdot \overrightarrow{E_m^*}(\overrightarrow{r}) \cdot \exp\left[i\left(\overrightarrow{k_l} - \overrightarrow{k_m}\right) \cdot \overrightarrow{r}\right] \tag{1}$$

where $\overrightarrow{E_l}(\overrightarrow{r})$ is the complex amplitude of the electric field vector of the lth plane wave and $\overrightarrow{k_l}$ is the corresponding wave-vector. Here each beam is considered as a plane wave in an interference area smaller than the spotsize of the beam. Eq. (1) gives a periodic light pattern in a real space. When a layer of photoresist is exposed to this interference pattern, a spatial periodic photoresist structure is formed after the development process. By replicating this photoresist structure with a high index material, one obtains a photonic crystal. The symmetry of the unit cell of the resultant photonic crystal is determined by the relation among the dot products of polarization vectors, i.e., $\overrightarrow{E_l}(\overrightarrow{r}) \cdot \overrightarrow{E_m^*}(\overrightarrow{r})$ $(1 \le l < m \le N)$. The lattice of the photonic crystal is determined by the reciprocal lattice vectors $\left(\overrightarrow{k_l} - \overrightarrow{k_m}\right)$ $(1 \le l < m \le N)$. In the present paper, we introduce a rational and systematical method for the design of photonic bandgap structures with some basic symmetries. We illustrate the present method with some 2D photonic crystals of triangular lattice and 3D photonic crystals of fcc lattice as examples.

2.1.1. 2D photonic crystals of triangular lattice

Three beams with wave-vectors $\overrightarrow{k_1} = \frac{2\pi}{\lambda}[-\sin\alpha, 0, \cos\alpha]$, $\overrightarrow{k_2} = \frac{2\pi}{\lambda}\left[1/2\sin\alpha, -\sqrt{3}/2\sin\alpha, \cos\alpha\right]$, $\overrightarrow{k_3} = \frac{2\pi}{\lambda}\left[1/2\sin\alpha, \sqrt{3}/2\sin\alpha, \cos\alpha\right]$ are combined to achieve a primitive reciprocal lattice corresponding to a real space interference pattern of triangular lattice. The wave-vector of each beam makes an angle of α with the z-axis. It then follows from Eq. (1) that

$$\begin{aligned} I(x,y) &= c_0 + 2c_{12}\cos\left[\frac{4\pi}{\sqrt{3}a}\left(x\sqrt{3}/2 - y/2\right)\right] \\ &\quad + 2c_{13}\cos\left[\frac{4\pi}{\sqrt{3}a}\left(x\sqrt{3}/2 + y/2\right)\right] + 2c_{23}\cos\left[\frac{4\pi}{\sqrt{3}a}y\right] \end{aligned} \tag{2}$$

where $a = 2\lambda/(3\sin\alpha)$ is the lattice constant, $c_0 = \left|\overrightarrow{E_1}\right|^2 + \left|\overrightarrow{E_2}\right|^2 + \left|\overrightarrow{E_3}\right|^2$, and $c_{lm} = \overrightarrow{E_l} \cdot \overrightarrow{E_m^*}$, $1 \le l < m \le 3$. In the present paper we only consider the case when $\overrightarrow{E_l} \cdot \overrightarrow{E_m^*}$ $(1 \le l < m \le N)$ are real (this is true for structures with a center of inversion).

After exposing a layer of photoresist to this interference pattern, the binarization in the photoresist development process gives a 2D triangular periodic photoresist structure. This layer of photoresist then serves as a mask to etch a substrate of high index to obtain a 2D triangular photonic crystal. In our numerical example, the dielectric constant of areas where $I(x,y) > I_t$ is assumed to be 1.0 (air) and that of the other areas to be 13.6 (GaAs). Generally speaking, the pattern or motif within the unit cell is determined by the threshold I_t and the values of c_{lm}, so does the photonic bandgap (photonic bandgap structures were searched by varying I_t in e.g. , [15]).

To maintain some basic symmetry of the photonic crystals (and similar features of the band structures), we should keep some relation among the constants c_{lm} $(1 \le l < m \le N)$. We then

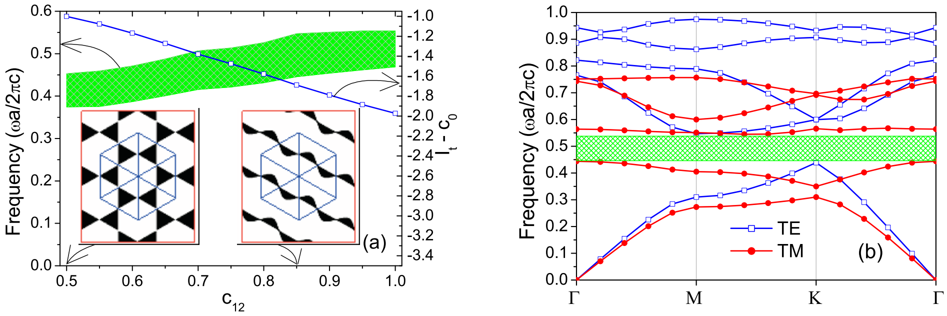

Fig. 1. (a) Maximal absolute photonic bandgap between bands 3 and 4 and the corresponding threshold I_t when c_{12} increases from 0.5 to 1.0. The other parameters are fixed as $c_{13} = c_{23} = 0.5$. The two insets are the binarized patterns for $(c_{12} = 0.5, I_t = c_0 - 1.002)$ and $(c_{12} = 0.85, I_t = c_0 - 1.6886)$, respectively. (b) The band structures for both polarizations for the case of $(c_{12} = 0.85, I_t = c_0 - 1.6886)$.

search optimal photonic crystals with large bandgaps by adjusting only one or two of the constants c_{lm}. Such a searching can be easily done by a simple scanning. In this numerical example, we keep relation $c_{13} = c_{23}$ and vary the relative value of c_{12} (c_0 is related to the contrast of the interference pattern and will be considered in stage 2 below). For each set of (c_{12}, c_{13}, c_{23}), we search for the maximal absolute bandgap between two certain (fixed) bands by varying I_t (one can always tune I_t by controlling the exposure dose). Fig. 1(a) shows the maximal absolute bandgap between bands 3 and 4 and the corresponding threshold I_t when c_{12} increases from 0.5 to 1.0 ($c_{13} = c_{23} = 0.5$ is fixed). (Here the band structures are obtained by using the software developed in MIT [16]. The calculated band structures have also been verified with a fast plane-wave expansion method [17].) From Fig. 1(a) one sees that these structures have a very large bandgap for a wide variation range of c_{12}. This also indicates a good fabrication tolerance of these structures. The two insets in Fig. 1(a) are the binarized patterns for $(c_{12} = 0.5, I_t = c_0 - 1.002)$ and $(c_{12} = 0.85, I_t = c_0 - 1.6886)$, respectively. These structures have a common symmetry of point group *2mm* (having one 2-fold rotation axis perpendicular to the plane of the drawing and two orthogonal mirror lines). Fig. 1(b) shows the band structures (for both TE and TM polarizations) for the case of $(c_{12} = 0.85, I_t = c_0 - 1.6886)$. From this figure one sees that the photonic crystal of the right inset of Fig. 1(a) gives a very large complete bandgap with a relative gap width of 20.4% (with respect to the mid-frequency of the gap).

2.1.2. 3D photonic crystals of fcc lattice

One set of wave-vectors of the four beams that interfere to create a real-space fcc interference pattern are $\overrightarrow{k_1} = \frac{\pi}{a}[201]$, $\overrightarrow{k_2} = \frac{\pi}{a}[\bar{2}01]$, $\overrightarrow{k_3} = \frac{\pi}{a}[02\bar{1}]$, $\overrightarrow{k_4} = \frac{\pi}{a}[0\bar{2}\bar{1}]$ [7]. The corresponding interference pattern is

$$\begin{aligned} I(x,y,z) \quad = \quad & c_0 + 2c_{12}\cos\left[\frac{4\pi}{a}x\right] + 2c_{13}\cos\left[\frac{2\pi}{a}(x-y+z)\right] \\ & +2c_{14}\cos\left[\frac{2\pi}{a}(x+y+z)\right] + 2c_{23}\cos\left[\frac{2\pi}{a}(x+y-z)\right] \\ & +2c_{24}\cos\left[\frac{2\pi}{a}(-x+y+z)\right] + 2c_{34}\cos\left[\frac{4\pi}{a}y\right] \end{aligned} \tag{3}$$

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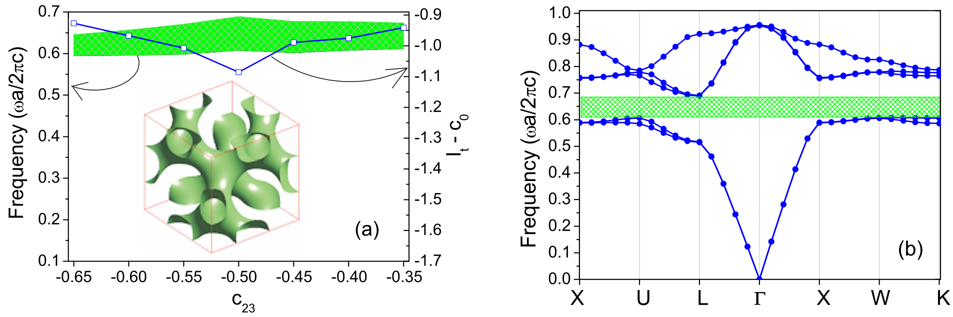

Fig. 2. (a) Maximal absolute photonic bandgap between bands 2 and 3 and the corresponding threshold I_t when c_{23} increases from -0.65 to -0.35. The other parameters are fixed as $c_{12} = c_{34} = 0$ and $c_{13} = c_{14} = c_{24} = 0.5$. The inset is the binarized pattern when $(c_{23} = -0.5, I_t = c_0 - 1.0859)$. (b) The band structure for the case of $(c_{23} = -0.5, I_t = c_0 - 1.0859)$.

where $a = \sqrt{5}\lambda/2$ is the lattice constant.

In such a 3D case the resultant resist structure should be replicated by infiltration [7] or electrodeposition [18] of a high index material. The refractive index of areas where $I(x,y,z) > I_t$ is assumed to be 1.0 (for air) and that of the other areas to be 2.5 (for titania or CdSe) in our numerical example. The 3D structure fabricated with the interference lithography must be completely connected within itself in order to prevent its collapse during the development stage. Thus, the threshold I_t cannot vary arbitrarily in the 3D case. For this example, we fix $c_{12} = c_{34} = 0$ and $c_{13} = c_{14} = c_{24} = 0.5$ to keep some basic symmetry, and leave c_{23} adjustable. Fig. 2(a) shows the maximal absolute bandgap between bands 2 and 3 and the corresponding threshold I_t when c_{23} increases from -0.65 to -0.35. The bandgaps shown in Fig. 2(a) indicate that these structures have a large bandgap for a wide variation range of c_{23}. The inset of Fig. 2(a) shows the binarized pattern for $(c_{23} = -0.5, I_t = c_0 - 1.0859)$. This structure has a symmetry of space group Fd$\bar{3}$m. Fig. 2(b) shows the corresponding band structure, from which one sees that this photonic crystal has a large complete bandgap with a relative gap width of 12.5%.

2.2. *Stage 2: Realization of the desired interference pattern*

All the constants c_{lm} $(1 \le l < m \le N)$ (however, not c_0) have been determined in the previous section in order to obtain a desired binarized interference pattern with a certain symmetry. In this section, we determine $\overrightarrow{E_l}(\overrightarrow{r})$ $(l = 1, 2, \ldots, N)$ from the required constants c_{lm} in order to realize the interference pattern. Meanwhile, the value of c_0 (corresponding to the background intensity of the total light) should be minimized in order to maximize the contrast of the pattern (the contrast is defined as $V = (I_{max} - I_{min})/(I_{max} + I_{min})$, where I_{min} is the minimal intensity, and I_{max} is the maximal intensity). Note that a minimal c_0 corresponds to a maximal V when all the constants c_{lm} $(1 \le l < m \le N)$ have been fixed.

Therefore, the realization of the interference pattern becomes how to minimize

$$c_0 = \left|\overrightarrow{E_1}\right|^2 + \left|\overrightarrow{E_2}\right|^2 + \cdots + \left|\overrightarrow{E_N}\right|^2 \tag{4}$$

subject to constrains

$$\overrightarrow{E_l} \cdot \overrightarrow{k_l} = 0, \; l = 1, 2, \ldots, N \tag{5}$$

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and

$$\overrightarrow{E_l} \cdot \overrightarrow{E_m^*} = c_{lm},\ 1 \le l < m \le N\ . \tag{6}$$

Such a nonlinear programming (NLP) problem with nonlinear constrains can be solved using the Sequential Quadratic Programming (SQP) method [19]. As a numerical example, here we consider the realization of the binarized interference pattern shown in the inset of Fig. 2(a). For this case, we have $c_{12} = c_{34} = 0$ and $c_{13} = c_{14} = -c_{23} = c_{24} = 0.5$ in Eq. (6). For linearly polarized beams, our SQP program gives the following solution

$$\begin{aligned}
\overrightarrow{E_1} &= [-0.2768, -0.6564, 0.5536], \\
\overrightarrow{E_2} &= [0.5667, 0.7170, 1.1335], \\
\overrightarrow{E_3} &= [-1.5880, 0.1340, 0.2681], \\
\overrightarrow{E_4} &= [0.0748, -0.2952, 0.5905].
\end{aligned} \tag{7}$$

The corresponding background intensity of the total light is $c_0 = 5.9871$ and the contrast of the interference pattern is $V = 0.4724$. For elliptically polarized beams, we found the following solution with our SQP program

$$\begin{aligned}
\overrightarrow{E_1} &= [-0.2320 + 0.2326i, 0.4047 + 0.4040i, 0.4640 - 0.4651i], \\
\overrightarrow{E_2} &= [-0.0856 - 0.3178i, -0.5478 + 0.1473i, -0.1711 - 0.6357i], \\
\overrightarrow{E_3} &= [-0.2551 + 0.9541i, 0.1836 + 0.0491i, 0.3673 + 0.0981i], \\
\overrightarrow{E_4} &= [-0.1837 - 0.0487i, -0.0843 + 0.3182i, 0.1686 - 0.6364i].
\end{aligned} \tag{8}$$

The corresponding background intensity of the total light is $c_0 = 3.4641$ and the contrast of the interference pattern is $V = 0.8165$. By comparing these two solutions, one sees that a better contrast can be obtained by using elliptically polarized beams for this example. (Note that the electric field vectors are different from those found in [10] and [20] for a similar structure.)

In an experiment of interference lithography, the energy ratio of the beams can be controlled according to the design by the beam splitting set-up. One then controls the total exposure dose (with the unit of mJ/cm^2) by controlling the intensity of the total input beam (with the unit of mW/cm^2) and the exposure time.

3. Conclusion

Interference lithography for the fabrication of a 2D or 3D photonic crystal with some desired symmetry has been considered. To maintain some basic symmetry of the photonic crystal, some relation among constants c_{lm} $(1 \le l < m \le N)$ has been kept when searching an optimal photonic crystal with a large bandgap. Constants c_{lm} are thus determined for the optimal photonic crystal. To create the corresponding interference pattern with certain symmetry and a maximal contrast, a nonlinear programming method has been used to find the optimal electric field vectors of the laser beams with a minimal c_0 from constants c_{lm} determined previously. Such a two-stage design method is different from a conventional design method, in which the electric field vectors are searched by directly maximizing the contrast of the pattern regardless of the symmetry of the unit cell of the photonic crystal. The present method provides an effective means for a rational and systematical design of new photonic crystals of good properties.

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