

# Translation of interference pattern by phase shift for diamond photonic crystals

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**Abstract:** We demonstrate the construction of diamond photonic crystal structures by the translation of a multi-beam interference pattern. Using phase shift of each beam, the double-exposed interference patterns can be aligned in the [111] direction for a face-centered cubic (FCC) and [210] direction for a body-centered cubic (BCC), respectively, producing diamond D from FCC and BCC-diamond like structure from BCC. The present result shows that the complete bandgap has been retained with slight deviation from ideal diamond symmetry.

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## 1. Introduction

Photonic crystals (PCs) are called a semiconductor of light and can be used to confine, manipulate and guide photons, which are desired for the next-generation optical circuits. Recently, multibeam interference lithography has been developed and holds promise in the PC fabrication over colloidal assembly,<sup>1</sup> direct writing,<sup>2-4</sup> and multi-layer process<sup>5</sup> because it produces 3D structure with controlled lattice and unit atoms in a large area by single exposure and is compatible with conventional photolithography.<sup>6</sup>

To date, among the proposed 3D PC structures, diamond networks have been known as the most optimized structure for having a large and complete photonic bandgaps (PBGs). Moreover, the PBG is robust enough to allow some structural modification within diamond symmetry,<sup>7</sup> This makes diamond structures especially attractive over other symmetries since it allows application of a wide range of approaches to fabricate them conveniently, including Yablonobite by direct drilling,<sup>8</sup> woodpile (<100>-diamond) by layer-by-layer fabrication,<sup>9</sup> <110>-diamond by layer-by-layer followed by reactive ion etching,<sup>10</sup> spiral diamond made by GLAD.<sup>11</sup> In the case of holographic lithography, it has been reported that four interfering beams can be assembled to create the level-set D (diamond) and G (gyroid) structures, and body-centered cubic (BCC) diamond.<sup>12-15</sup> All of these structures possess a PBG with larger than 20% between the 2nd and 3rd bands for a refractive index of  $n=3.6$ , close to the largest yet calculated.<sup>16</sup>

In this letter, we demonstrate the translation of 3D interference patterns to construct two types of diamond structures. Since the diamond symmetry can be alternatively achieved by two simple FCC or BCC sublattices, displaced along [111] direction or [210] direction, respectively, the superposition of the interference pattern and the shifted pattern could approximate the corresponding diamond structures. Specifically, we demonstrate phase-induced translation of simple FCC and BCC interference pattern. Then, we investigate the PBGs of two superimposed interference patterns of FCC and BCC, displaced in aforementioned directions. In practice, this method can be achieved by using double-exposure holographic lithography with phase shift to produce polymeric structures.<sup>17,18</sup> The double-exposure with phase shift is preferred over multiplexed holography because of the alignment process.<sup>19</sup> Compared to the previously reported results based on single-exposure of four-beam interference by controlling the polarization of each beam,<sup>13,14</sup> our method provide much improved contrast of the diamond interference. The high pattern contrast is crucial for

practical fabrication of photoresist structures with clearly defined and completely opened pores.<sup>20,21</sup> Furthermore, this method can be flexible by simply changing the intensity of each exposure, resulting in F43m from FCC interference pattern, which has two different PBGs.<sup>16</sup>

## 2. Translation of FCC or BCC interference patterns by phase shift

To construct 3D structures, four-beam interference has been widely used. The intensity distribution of the interference field of four mutually coherent laser beams can be described by Fourier superposition and can be written as

$$I = \sum_{n=1}^4 E_n^2 + \sum_{m<n}^4 E_n E_m |\boldsymbol{\varepsilon}_n \cdot \boldsymbol{\varepsilon}_m^*| \cos[(\mathbf{k}_n - \mathbf{k}_m) \cdot \mathbf{r} + (\phi_{n0} - \phi_{m0})]. \quad (1)$$

where  $E_n$ ,  $\boldsymbol{\varepsilon}_n$ ,  $\mathbf{k}_n$  and  $\phi_n$  are the amplitude, the unit polarization vector, the wave vector, and the phase of the  $n$ th beam, respectively. Here, we control the phase of each beam (i.e., relative phase difference) to shift the interference pattern in a certain direction. In experiment, the phase shift can be produced by phase retarders such as wave-plates,<sup>17</sup> Kerr cells and Pockels cells. When the relative phase difference in Eq. (1) is changed by  $(\phi_n - \phi_m)$ , the interference term,  $I_{nm}$  is described by

$$I_{nm} = E_n E_m |\boldsymbol{\varepsilon}_n \cdot \boldsymbol{\varepsilon}_m^*| \cos[(\mathbf{k}_n - \mathbf{k}_m) \cdot \mathbf{r} + (\phi_{n0} - \phi_{m0}) + (\phi_n - \phi_m)]. \quad (2)$$

Meanwhile, since the interference term translated by  $\mathbf{r}'$  in space can be described by,

$$I_{nm} = E_n E_m |\boldsymbol{\varepsilon}_n \cdot \boldsymbol{\varepsilon}_m^*| \cos[(\mathbf{k}_n - \mathbf{k}_m) \cdot (\mathbf{r} + \mathbf{r}') + (\phi_{n0} - \phi_{m0})]. \quad (3)$$

The relationship between the spatial translation in a certain direction and the phase shift can be obtained by comparing Eqs. (2) and (3) and given by

$$(\phi_n - \phi_m) = (\mathbf{k}_n - \mathbf{k}_m) \cdot \mathbf{r}'. \quad (4)$$

Then, the phase shift of each beam, which induces the translation of the interference pattern, can be determined by Eq. (4) of each interference term.

First, we consider the translation of the simple FCC interference pattern with  $Fm\bar{3}m$  space group.<sup>22</sup> This structure has been demonstrated with four beams: one set of two coplanar beams interfere with another set whose plane is perpendicular to the first. This requires a substrate that is transparent at the light's wavelength and a prism to compensate for the refraction at the air-photoresist interface.<sup>22</sup> When the initial phase of each beam is set at zero in Eq. (2), the interference pattern can be expressed as:

$$I_{nm} \sim \cos[2\pi/d(x-y+z) + (\phi_1 - \phi_3)] + \cos[2\pi/d(x+y+z) + (\phi_1 - \phi_4)] \\ + \cos[2\pi/d(-x-y+z) + (\phi_2 - \phi_3)] + \cos[2\pi/d(-x+y+z) + (\phi_2 - \phi_4)] \quad (5)$$

where  $d$  is the lattice constant. In order to translate the interference pattern in [111] direction by  $\beta d/4\pi$  as shown in Fig. 1(a), phase differences are calculated from Eq. (4) and given by  $(\phi_1 - \phi_3) = \beta$ ,  $(\phi_1 - \phi_4) = 3\beta$ ,  $(\phi_2 - \phi_3) = -\beta$ , and  $(\phi_2 - \phi_4) = \beta$ . Then, the phases of four beams relative to the initial zero value are  $\phi_1 = 3\beta$ ,  $\phi_2 = \beta$ ,  $\phi_3 = 2\beta$ , and  $\phi_4 = 0$ .

For BCC interference pattern, the beam configurations for  $m\bar{3}m$  symmetry of the unit atoms are described as:

$$I_{nm} \sim \cos[4\pi/d(y+z) + (\phi_1 - \phi_2)] + \cos[4\pi/d(x+y) + (\phi_1 - \phi_3)] \\ + \cos[4\pi/d(x+z) + (\phi_1 - \phi_4)] + \cos[4\pi/d(x-z) + (\phi_2 - \phi_3)] \\ + \cos[4\pi/d(x-y) + (\phi_2 - \phi_4)] + \cos[4\pi/d(-y+z) + (\phi_3 - \phi_4)] \quad (6)$$

which has an  $\text{Im}\bar{3}m$  space group of the BCC lattice. Likewise in the FCC, the translation of the interference pattern by  $\beta d/4\pi(2,1,0)$  (see Fig. 1(b)) can be achieved by solving Eq. (2). The phase differences are given by  $(\phi_1 - \phi_2) = \beta$ ,  $(\phi_1 - \phi_3) = 3\beta$ ,  $(\phi_1 - \phi_4) = 2\beta$ ,  $(\phi_2 - \phi_3) = 2\beta$ ,  $(\phi_2 - \phi_4) = \beta$ , and  $(\phi_3 - \phi_4) = -\beta$ . Finally, the phases of four beams relative to the initial zero value are  $\phi_1 = 3\beta$ ,  $\phi_2 = 2\beta$ ,  $\phi_3 = 0$ , and  $\phi_4 = \beta$ .

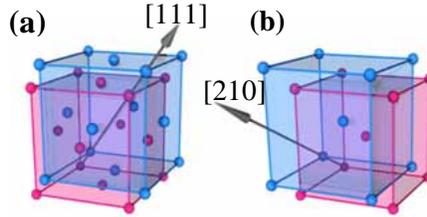


Fig. 1. Translation of (a) FCC interference pattern in the [111] direction and (b) BCC interference in the [210] direction.

### 3. Superimposition of interference patterns with phase shift

With these pattern shifts, the double-exposed interference patterns can be described by the superposition of all exposed patterns. Figs. 2(a), 2(b) and 2(c) show the relative position of two FCC lattices (red for the initial pattern and blue for the shifted one), described by Eq. (5) for  $\beta = 0.80\pi$ ,  $1.00\pi$  and  $1.16\pi$ , respectively. Then, the translations are  $0.20d$ ,  $0.25d$  and  $0.29d$ , all in [111] direction. The level surfaces of the double-exposed FCC interference patterns are reproduced in Figs. 2(d)-2(f) for their respective cases.

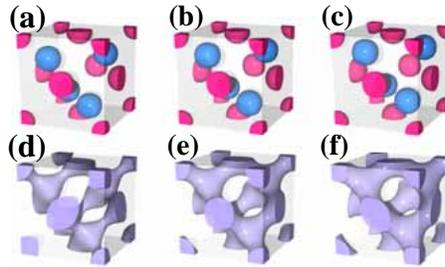


Fig. 2. The relative position of the FCC interference pattern (red) and the shifted pattern (blue) in the [111] direction by (a)  $0.20d(1,1,1)$ , (b)  $0.25d(1,1,1)$ , and (c)  $0.29d(1,1,1)$ . The level surface of each double-exposed FCC interference pattern with a filling fraction of 0.22 is shown in (d-f) for their respective cases.

Remarkably, overall exposures make a local connection between the atoms formed in each exposure. For the FCC, the superposition of interference patterns with the translation by  $0.25d$  describes the level surface of diamond D structure (see Fig. 2(e)) and given by

$$\begin{aligned}
 I_{nm} \sim & \cos\left[\frac{2\pi}{d}(x-y+z)\right] + \cos\left[\frac{2\pi}{d}(x+y+z)\right] \\
 & + \cos\left[\frac{2\pi}{d}(-x-y+z)\right] + \cos\left[\frac{2\pi}{d}(-x+y+z)\right] \\
 & + \sin\left[\frac{2\pi}{d}(x-y+z)\right] - \sin\left[\frac{2\pi}{d}(x+y+z)\right] \\
 & - \sin\left[\frac{2\pi}{d}(-x-y+z)\right] + \sin\left[\frac{2\pi}{d}(-x+y+z)\right]
 \end{aligned} \tag{7}$$

It is noteworthy that this equation contains 8 terms instead of 4 terms reported in the literature in describing the same type of diamond D. These additional terms provide higher contrast of the interference pattern.<sup>7,14</sup> Considering the intensity profile along [111] direction (see Fig. 3), the contrast defined by difference between maximum and minimum intensities is

8 for 8-term D in contrast to  $4\sqrt{2}$  for 4-term D. In practical applications of interference lithography, low contrast interference cannot produce well-defined photoresist pattern with completely opened, porous structure due to the homogeneous background of acid generation.<sup>20</sup>

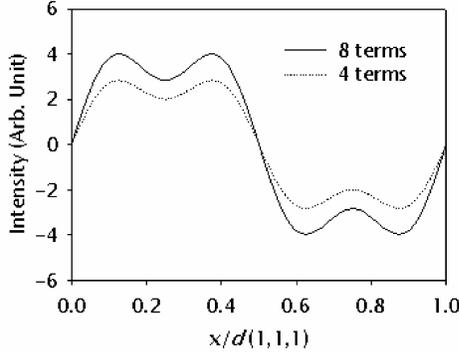


Fig. 3. Intensity profile of 8-term and 4-term interference patterns along [111] direction

Meanwhile, instead of diamond D, this method can simply construct  $\overline{F43m}$ , with the different intensity of each exposure, which possesses dual complete PBGs.<sup>14</sup>

In Figs. 4(a), 4(b) and 4(c), the position of two BCC lattices (red for the initial pattern and blue for the shifted one), described by Eq. (6) are shown for  $\beta = 0.40\pi$ ,  $0.50\pi$  and  $1.16\pi$ , respectively. Then, the translations are  $0.20d$ ,  $0.25d$  and  $0.29d$ , all in [210] direction.

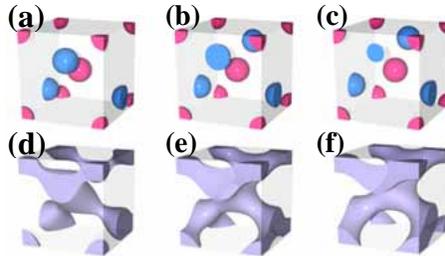


Fig. 4. The relative position of the BCC interference pattern (red) and the shifted pattern (blue) in the [210] direction by (a)  $0.20d(1,1,1)$ , (b)  $0.25d(1,1,1)$ , and (c)  $0.29d(1,1,1)$ . The level surface of each double-exposed BCC interference pattern with a filling fraction of 0.20 is shown in (d–f) for their respective cases.

The level surfaces of the double-exposed BCC interference patterns are reproduced in Figs. 4(d)–4(f) for their respective cases. For the BCC-based structure, shift of interference pattern into [210] by  $0.25d$  constructs a BCC diamond-like structure with diamond D symmetry in the body-centered tetragonal unit cell (see Fig 4(e)).<sup>7</sup> From Eq. (6), the level surface of this structure can be expressed by

$$\begin{aligned}
 I_{nm} \sim & \cos\left[4\pi/d(x+y)\right] + \cos\left[4\pi/d(y+z)\right] \\
 & + \cos\left[4\pi/d(-y+z)\right] + \cos\left[4\pi/d(x-y)\right] \\
 & + \sin\left[4\pi/d(x+y)\right] - \sin\left[4\pi/d(y+z)\right] \\
 & - \sin\left[4\pi/d(-y+z)\right] - \sin\left[4\pi/d(x-y)\right]
 \end{aligned} \tag{8}$$

#### 4. Bandgap of superimposed FCC and BCC interference patterns

In Fig. 5, we calculate the PBG of the double-exposed FCC as a function of the degree of phase shift. The polymeric structure by interference lithography can be used as a template to deposit high refractive index materials.<sup>23</sup> The PCs with a refractive index of 3.45 produced

from FCC-based structure show a complete PBG between the 2nd and 3rd bands. The volume fraction is optimized to achieve a maximum PBG at each point, ranging from 0.22 to 0.26. The bandgap width has a local maximum at a translation of  $0.25d(1,1,1)$  with diamond D symmetry defined in Eq. (6). They show a complete PBG with the gap-midgap ratio as large as 25%, which is comparable to the previous results.<sup>12</sup> Meanwhile, the complete PBG appears when the degree of the pattern translation is varied from 0.18 to 0.30. The relatively large PBG is retained within the deviation from diamond D (See Fig 3, these structures possess the PBG width above 10%). Therefore, this method is feasible even with the experimental error during translation. Likewise the FCC case, we calculate PBG of BCC-based structure as shown in Fig. 5. The optimized volume fraction for a maximum PBG is found 0.20 for the normalized pattern shift of 0.25, and the optimal volume fraction is increased to 0.30 for the upper and lower bounds of the phase shift in Fig. 5. The bandgap width reaches a maximum, at which the gap-midgap ratio is 22%, for a translation of  $0.25d(2,1,0)$  with BCC diamond-like structure defined in Eq. (8).<sup>15</sup>

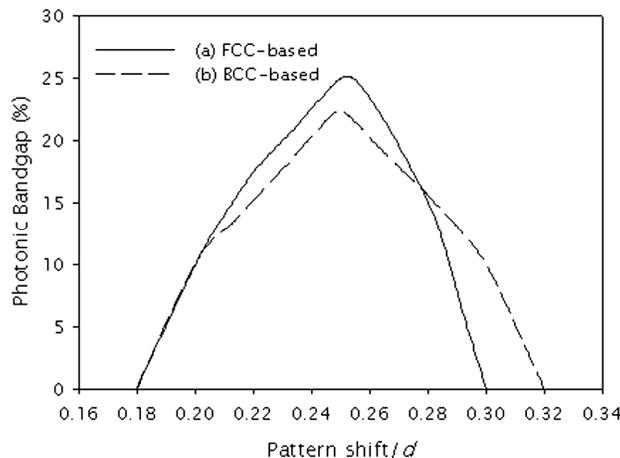


Fig. 5. Complete PBG of double-exposed (a) FCC and (b) BCC interference patterns as a function of the normalized pattern shift in [111] and [210], respectively.

#### 4. Conclusion

In summary, we propose a double exposure technique that translates interference patterns by phase shift. The superposition of two interference patterns constructs partially overlapped structures, whereas the two unit atoms in the basis are connected with each other. We demonstrate that translation in both the [111] direction for FCC and the [210] direction for BCC, respectively, can produce diamond D and BCC diamond-like structure, respectively. Such structures show a large complete PBG between 2nd and 3rd bands, in agreement with the literature results. The large bandgap is retained within the accepted variation in the degree of translation. Compared to the single-exposed diamond D structures, the present double-exposed structure has a better contrast of the interference pattern, which is necessary to their practical realization in interference lithography.

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