Calculation of photonic bandgap for 2D hexagonal and square structure base on hybrid polymer material

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Abstract. We have calculated 2D photonic crystal band gap using plane-wave expansion method. The studied model of structures is hexagonal lattice and square lattice of rod cylinder in air. We have simulated the dispersion relation of it structure using hybrid polymer as rod material. The parameter structures are $n_{\text{rod}}=1.5$, $n_{\text{hole}}=1$, and $r_{\text{rod}}=0.25a$, where $a$ is lattice constant. We found the distributed feedback occurs at the edge of upper band or frequency at $0.66 \ (a/\lambda)$. In our experimental work, we have successfully fabricated the 2D photonic crystal from hybrid polymer incorporated with organic dye laser. The lasing characteristics were investigated using strip-line excitation light of SHG Nd-YAG laser ($\lambda=532 \text{ nm}$). The lasing wavelengths for hexagonal structure are observed at 606 nm and 621 nm for photonic crystal period of 400 nm and 410 nm, respectively. $\lambda=532 \text{ nm}$. Whereas the square structure, the lasing wavelengths are observed at (588 nm ± 2) and (606 nm ± 2 nm) for grating period of 391 nm and 405 nm.

1. Introduction
Photonic crystals have photonic bandgap which able to control the flow of electromagnetic radiation or able to modify light-matter interaction [1]. The photonic bandgap or dispersion relation between photon energy and wave vector is useful for realization of various new optical devices. In the experimental field, much effort has been exerted to develop optical devices in order to realization the integrated optical circuit. Some transparent materials have been developed such as inorganic glasses and organic polymer. Inorganic glasses have some disadvantages for optical and optoelectronic devices since they have low flexibility and need high temperature for processing. On the other hand, utilizing the organic polymers in optical devices can overcome some of the disadvantages of inorganic glasses, but they exhibit a low heat resistance and poor adhesion in some substrate [2].

In this paper, we have reported the calculation result of bandgap of 2D photonic crystal using hybrid polymer as base material. The method of calculation is plane-wave expansion using infinite model of 2D photonic crystal. The model of structures is hexagonal lattice and square lattice of rod cylinder in air which hybrid polymer as rod material. Furthermore, we report the fabrication result of 2D photonic crystal from hybrid polymer incorporated with organic dye-laser. Finally, we describe the correlation between computational and experimental results by observation the lasing action.
2. Methods

The characteristics of photonic crystal can be known from the photonic band structures. The band structures give information about radiation behavior when propagating within the specific direction inside the photonic crystal [1,2]. Using the band structure, the parameter values of the photonic crystal can be determined for each application. In this paper, we calculated the photonic band structures using plane wave expansion (PWE) method.

The main problem of band structure computation is finding the dispersion relation of photonic crystal. The dispersion relation can be determined by solve the eigen problem of Helmholtz equation inside the periodic structures. For TM polarization case of 2D photonic crystal with non-dispersive medium, the eigen problem of Helmholtz equation is written as follows [3].

\[
\frac{\partial^2}{\partial x^2} + \frac{1}{\varepsilon(x,y)} \frac{\partial}{\partial y} + \frac{1}{\varepsilon(x,y)} \frac{\partial^2}{\partial y^2} \bar{H}_n(\bar{r}) = \frac{\omega^2}{c^2} \bar{H}_n(\bar{r})
\]  

(1)

Here, \(c\) denotes the vacuum speed of light and \(\bar{r} = (x, y)\) denotes a 2D vector in coordinate space. The dielectric constant \(\varepsilon(\bar{r}) = \varepsilon(\bar{r} + \bar{R})\) contains all the structural information of the photonic crystal. Equation (1) represents a differential equation with periodic coefficients. Therefore, the solution of its equation obeys to the Bloch-Floquet theorem. The structures have translational symmetry; therefore, the solution is labelled with a wave vector \(\mathbf{k}\) in Brillouin zone of the reciprocal lattice. The eigen modes corresponding to the eigen frequency \(\omega_n(\mathbf{k})\), where \(n\) is discrete band index. The eigen modes or Bloch function can be represented in the form as follows [4].

\[
\bar{H}_n(\bar{r}) = \bar{H}_{kk}(\bar{r}) \cdot \exp\left(j \cdot \mathbf{k} \cdot \bar{r}\right)
\]  

(2)

In this case, \(\bar{H}_{kk}(\bar{r} + \bar{R}) = \bar{H}_{kk}(\bar{r})\) is periodic with the photonic crystal lattice. A simple way for solving equation (1) and (2) is to expand all the periodic function into a Fourier series over reciprocal lattice vector \(\bar{G}\). Thus, we can represent the wave function in wave vectors space as follow:

\[
\bar{H}_n(\bar{r}) = \bar{H}_{kk}(\bar{r}) = \sum_{\bar{G}} \bar{H}_{kk}(\bar{G}) \exp\left(j \cdot \bar{G} \cdot \bar{r}\right)
\]  

(3)

In the same way, the dielectric function can also be expanded to the Fourier series due to the periodicity as follows,

\[
\frac{1}{\varepsilon(\bar{r})} = \sum_{\bar{G}} \kappa(\bar{G}) \exp(i\bar{G} \cdot \bar{r})
\]  

(4)

where \(\kappa(\bar{G})\) are Fourier expansion coefficients which depend on the reciprocal lattice vectors. The Fourier expansion coefficients \(\kappa(\bar{G})\) is given by,

\[
\kappa(\bar{G}) = \frac{1}{V_0} \int_{V_0} d\bar{r} \frac{1}{\varepsilon(\bar{r})} \exp(-i\bar{G} \cdot \bar{r})
\]  

(5)

where \(V_0\) corresponds to the volume of the photonic crystal unit-cell.

In order to compute the integral in equation (5), for case of 2D dielectric rods is convenient to use polar coordinate system. The calculation of the integral in equation (5) can obtain the Fourier expansion coefficients as follows [4,5],

\[
\kappa(\bar{G}) = 2J_1(G|\bar{r}_o|) \frac{1}{\varepsilon_0 - \varepsilon_\rho} \frac{1}{G|\bar{r}_o|}
\]  

(6)
Here, $J_1(G|\rho|)$ is the first order of Bessel function and $f = \varepsilon V \rho$ is cross-section area between the rod and the total 2D volume of the unit cell.

In our experiment, two dimensional gratings were fabricated from hybrid polymer incorporated with organic dye laser DCM using Lloyd mirror interference method. The photo-polymerization processes dependent on the dose of laser and the irradiation time. In this experiment, the dose of laser was varied in three kinds, i.e. 120 mWatt, 200 mWatt, and 320 mWatt with same irradiation time at ¼ second. Fabrication the gratings at the dose of laser 120 mWatt did not generate. It caused by the photopolymerization process did not occur when the dose of laser less than the threshold. In this case, the cross linking in organic side chain could not formatted. The film of precursor hybrid polymer remained in the gel phase and dissolved when etching process was conducted. Whereas if the dose of laser much more than the threshold, the grating will formed in one shoot, and the second shoot did not effect on grating formation.

3. Results and Discussion
In a 2D system, computation of the band structure would begin from the canter of Brillouin zone, designated by the letter $\Gamma$, which has a wave vector that is equals to zero. Computation is then carried out to the $M$ point, $K$ point, and back to the $\Gamma$ point, in the case of hexagonal lattice, or to the $M$ point, $X$ point, and return to the $\Gamma$ point, in the case of square lattice. The contour obtained by the connection of the symmetry points is called k-path. The k-path for 2D photonic crystal with hexagonal lattice is shown in Figure 1.

The resulting path are represented in a $(k_x, k_y, \omega)$ coordinate system. In the plot, symmetry points lie along horizontal axis and the frequency lies along vertical axis, as shown in Figure 2 and Figure 3. The graph in Figure 2 and Figure 3 show the simulation results of dispersion relation of 2D hexagonal and 2D square structure using hybrid polymer as rod material. The parameter structures were assumed as follow: $n_{rod} = 1.5$, $n_{hole} = 1$, and $r_{rod} = 0.25a$, where $a$ is lattice constant.
Inside a photonic crystal, the characteristics of a light wave propagation will change. Around the eigen mode of the photonic crystal, the concentration of propagation mode will increase due to the decrease the group velocity. Exactly on the eigen band, the process of distributed feedback will occur, due to zero group velocity [6]. Therefore, the stimulated emission will increase at the edge of the photonic band, when the group velocity equal to zero [7].

According to the graph in Figure 2 and Figure 3, we can obtain that the distributed feedback occurs at the edge of the upper band, or at the frequency of 0.66 (a/λ), where a and λ are the lattice constant and the lasing wavelength, respectively. The emission spectra of DCM lies in the range between 530 nm and 660 nm [7]. When we substituted these values into the previous frequency relation, we obtain that the photonic crystal periods for lasing application lies in the range of 350 nm and 435 nm.

![Figure 2. Photonic band gap of 2D hexagonal structure](image1)

![Figure 3. Photonic band gap of 2D square structure](image2)

We would like to study the predicted lasing action on a sample made from hybrid polymer incorporated with organic dye laser (DCM). The sample are optically pumped using SHG of Nd-YAG laser at 532 nm. When the pumping power is less than the pumping threshold, we observe amplified spontaneous emission (ASE) spectrum. The ASE spectrum will sharpen as we increase the pumping power. When the pumping power is higher than power threshold, the lasing action started to occur. For both photonic-crystal periods, the power thresholds are around 10 mJ/pulse.cm². We can observe the

![Figure 4. Lasing action for hexagonal structure.](image3)

![Figure 5. Lasing action for square structure](image4)
lasing action at 606 nm and 621 nm for hexagonal structure respectively as shown in Figure 4. Whereas for square structure, the lasing wavelengths are observed at 588 nm and 606 nm for grating period of 391 nm and 405 nm as shown in Figure 5.

4. Conclusion
We have performed a calculation of the dispersion relation based on the infinite model for a 2D photonic crystal with hexagonal lattice. This result can be used to study the lasing action of a 2D photonic crystal that were made from hybrid polymers incorporated with organic dye-laser (DCM). The lasing action arises from 2D distributed feedback of hexagonal structures, which according to our simulation occurs at K point or at the edge of photonic band where the group velocity is equal to zero. The results of our simulation agree quite well with the observed lasing in hexagonal structure action at 606 nm and 621 nm with period of 400 nm and 410 nm, respectively. The lasing wavelengths are observed in the square structure occurs at 588 nm and 606 nm with period of 391 nm and 405 nm.

5. References
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