Simulation Computation of Two-dimensional Hexagonal Honeycomb Photonic Crystals Energy Band Structure Based on COMSOL

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Abstract. This study employs COMSOL software, integrating the plane wave expansion method and finite element method, to simulate and analyze the energy band structure of two-dimensional hexagonal honeycomb photonic crystals. By setting parameters and conducting scans, this paper not only maps out the electric field intensity and energy band distribution but also discovers a significant enhancement of electric field intensity at the lattice's high symmetry points, indicating a higher likelihood of electromagnetic waves' presence at these points. Furthermore, the notable energy gaps between the second and third energy bands provide directions for subsequent research. The findings of this study are of significant value for research and development in optoelectronic integration and communication, demonstrating an effective comprehensive method for analyzing the energy band structure of two-dimensional hexagonal honeycomb photonic crystals.

Keywords: Photonic crystals, Energy band structure, FEM.

1. Introduction

With the rapid development of science and technology and the arrival of the information age, people have higher and higher requirements for electronic technology and electronic products, and the traditional electronic field has been unable to meet the demands of the development of high-end technology. Therefore, photonic technology has become an important research object in the field of information technology. Compared with electrons, photons are stronger and faster in storage capacity, information load, information transmission and processing capabilities, but photons are difficult to be controlled. therefore, the search for a new type of controllable photon structure has become the main research content of physicists. In the 1980s, a special crystal with not only energy bands and defect states but also photonic bandgap and photonic localized characteristics was proposed, that is, photonic crystals. In the 1990s, Russell put forward the concept of photonic crystal fiber (Photonic Crystal Fiber, PCF)[1].

Comprising spatially periodic structures, photonic crystals are constructed from multiple materials with differing dielectric constants, essentially serving as dielectrics. In the past few decades, photonic crystals can be used to control light [2]. Furthermore, the remarkable achievements in managing electromagnetic wave transmission and interaction with materials are significantly represented by photonic crystals. The manipulation of light flow through photonic crystals with nontrivial bandgaps has garnered extensive interest, highlighting the possibilities with engineered metamaterials, including the innovative left-handed media recently identified[3]. Continuous studies revealed that making further researches on the photonic crystals is of great significance. The in-depth study of photonic crystals will contribute to the application and development of optoelectronic integration and optoelectronic communication [4-6]. According to the dimensions, photonic crystals can be divided into two-dimensional and three-dimensional. This paper mainly discusses the calculation and simulation of two-dimensional.

Through the photonic crystal, the modulation of electromagnetic waves by Bragg diffraction results in the formation of an energy band structure, known as photonic bands, along with potential gaps known as photonic band gaps (PBG). Electromagnetic waves with frequencies within the

photonic energy band can propagate almost losslessly through the photonic crystal, whereas electromagnetic waves at the frequencies of the photonic band gap cannot propagate within the photonic crystal. In the region where the band gaps of TE and TM waves coincide, it is called absolute band gap or complete band gap. Typically, a photonic crystal's performance stability increases with the broadening of its band gap [7-8]. Popular techniques for analyzing photonic crystals include the plane wave expansion, finite element, transfer matrix, and finite-difference time-domain methods [2,9,10]. These methods have their own advantages and disadvantages.

This paper makes a comprehensive consideration of intuition and applicability, combined with the plane wave expansion method, the energy band structure and electric field intensity diagram of two-dimensional hexagonal photonic crystals are studied by COMSOL Multiphysics software based on finite element method, which brings convenience for further research and application of photonic crystals.

2. Research methods

2.1. Plane wave expansion

The plane wave method fundamentally operates by expressing the material's density and elastic constants as a Fourier series through the superposition of plane waves in reciprocal vector space. This transforms the light wave equation into an eigenvalue equation, from which the dispersion relationship is derived by solving for the eigenvalues.

Reference [11] provides a detailed derivation of the Fourier transform for the dielectric constant of two-dimensional photonic crystals, with its formula being detailed.

$$\varepsilon^{-1}(G_{\parallel}) = \begin{cases} \frac{1}{\varepsilon_b}(1-f) + \frac{2f}{r_a^2}\int_0^{r_a} r\frac{1}{\varepsilon_a(r)}dr \ (G_{\parallel}=0) \\ \frac{2f}{r_a^2}\int_0^{r_a} r\frac{1}{\varepsilon_a(r)}J_0 G_{\parallel}dr - \frac{2f}{\varepsilon_b}\frac{J_1(G_{\parallel}a)}{G_{\parallel}a} \ (G_{\parallel}\neq 0) \end{cases} \quad (1)$$

Using the plane-wave expansion method, the eigenvalue equations for TE waves are derived.

$$\sum_{\vec{G'}}\left|\vec{K}+\vec{G'}\right|\left|\vec{K}+\vec{G}\right|\varepsilon^{-1}\left(\vec{G}-\vec{G'}\right)E_k\left(\vec{G'}\right) = E_k\left(\vec{G'}\right) = \frac{\omega^2}{c^2}E_k\left(\vec{G}\right) \quad (2)$$

2.2. Finite Elements Method (F.E.M)

The finite element method (Finite Element Method, F.E.M) is to divide the continuous field solution into finite discrete sub-domain element regions, and use a simple function to approximate the field value in each discrete sub-element, and then combine the field values of all elements to approach the solution of the whole field [9]. By integrating Bloch theory with Maxwell's equations that dictate electromagnetic wave propagation, the Finite Element Method (FEM) simplifies the complex band diagram issues into manageable eigenvalue problems. This is achieved by resolving the eigenvalue in relation to the wave vector K and frequency. The Maxwell equations, which govern the propagation of electromagnetic waves and are combined with Bloch theory, are transformed by the Finite Element Method (FEM) from complex band diagram problems into simpler eigenvalue equations. This transformation involves solving the eigenvalues with respect to the wave vector K across different frequencies [12].

In this study, utilizing COMSOL Multiphysics software and guided by Bloch theory and Floquet periodic boundary conditions, we transform the periodic structure's finite element discrete characteristic equation into a complex coefficient characteristic equation within a singular periodic unit cell, thereby deriving the dispersion curve. To specify, in COMSOL, following Bloch's theorem, we craft the crystal's fundamental single-cell structure with geometric tools. We apply two periodic boundary conditions to its quadrilateral perimeters, establishing an optimal mesh network. Subsequently, by defining the range of wave vector $\vec{k}$, we deduce the energy band and electric field

intensity diagrams for the two-dimensional hexagonal photonic crystal, streamlining the complexity into concise visual representations $\vec{k}$.

3. Numerical calculation and simulation results

3.1. The establishment of simulation model

In this paper, we focus on the two-dimensional hexagonal photonic crystal due to its periodic structural characteristics. Given the periodic nature of the photonic crystal, we have selected a single unit cell of the crystal as the basis for our calculations.

Figure 1 shows a unit cell of a two-dimensional photonic crystal with hexagonal structure, which is composed of two equilateral triangles. The side length of the equilateral triangle is a, and the two basis vectors are$\overrightarrow{a_1}$、$\overrightarrow{a_2}$, $\overrightarrow{a_1} = (a, 0)$, $\overrightarrow{a_2} = (-\frac{a}{2}, -\frac{\sqrt{3}}{2})$, $\overrightarrow{a_3} = (-\frac{a}{2}, -\frac{\sqrt{3}}{2})$,inverted lattice vector are $\overrightarrow{b_1} = 2\pi\frac{\overrightarrow{a_2}\times\overrightarrow{a_3}}{\overrightarrow{a_1}\cdot(\overrightarrow{a_2}\times\overrightarrow{a_3})} = \frac{2\pi}{a}(\vec{\imath} - \frac{1}{\sqrt{3}}\vec{\jmath})$, $\overrightarrow{b_2} = 2\pi\frac{\overrightarrow{a_1}\times\overrightarrow{a_3}}{\overrightarrow{a_2}\cdot(\overrightarrow{a_1}\times\overrightarrow{a_3})} = \frac{2\pi}{a}\frac{2}{\sqrt{3}}\vec{\jmath}$, based on this, Brillouin zone is drawn.In figure 2, the blue region is a reduced Brillouin zone defined by three high symmetry points, Γ、M、K , and the coordinates of the three points are $\vec{\Gamma} = (0,0)$、$\vec{K} = \left(\frac{2\pi}{3a}, \frac{2\sqrt{3}\pi}{3a}\right)$、$\vec{M} = \left(0, \frac{2\sqrt{3}\pi}{3a}\right)$,$k_x$, k_y are the component of Bloch wave vector $\vec{K}$.

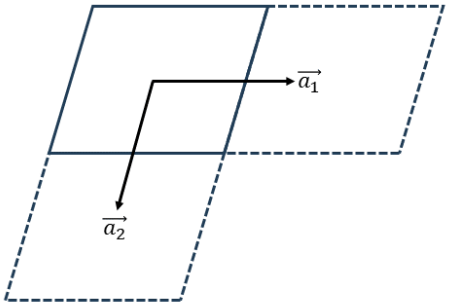


Figure 1. Define the lattice vector of a hexagonal unit cell $\overrightarrow{a_1}$、$\overrightarrow{a_2}$

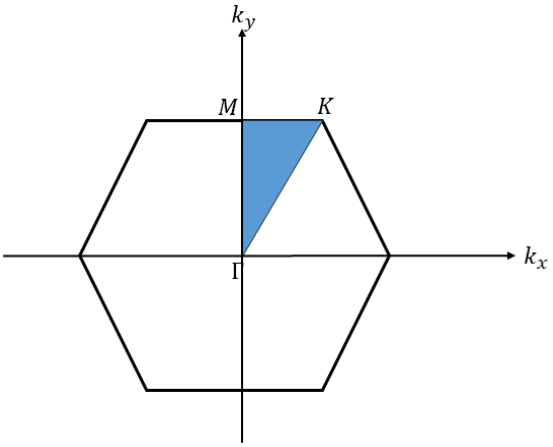


Figure 2. The first Brillouin zone

Parameter number settings: a=1um, b=0.5um, kx=0, ky=0, px=2*pi/3/a, py=px*sqrt(3), n_pos=1, n=13, kx = px, ky = py.

Geometric construction: simplify the geometric construction of the hexagon to the simulation of the parallelogram, construct a parallelogram with a side length of 1 meter, and make a parallelogram with a side length of 0.5 meters. the dielectric constant of the material of the inner parallelogram is set to 13, the gap between the two parallelograms is vacuum, and the dielectric constant is 1.

Setting of boundary conditions: floquet periodic boundary conditions.

Parameterized scan settings:kx=1.0e-4^range(1,n) range(0,(px-0)/(n-1),px) range(px,(0-px)/(n-1),0),ky= range(0,(py-0)/(n-1),py) py*1^range(1,n) range(py,(0-py)/(n-1),0), range(1,1,n) range (n,1,2*n-1) range(2*n-1,1,3*n-2).Characteristic frequency search reference value is Hz.

In the two-dimensional photonic crystal structure, the Bloch wave vector is limited to the first Brillouin zone and moves along the boundary of the first Brillouin zone (Γ-X-M). Here, the first Brillouin zone is divided into three parts to simulate (Γ-X), (X-M), (Γ-M), which can be seen from the above results. The results calculated by the mathematical model derived in this paper are basically consistent with the results obtained by the traditional method in the literature.

3.2. simulation results

Once parameters have been established, COMSOL software conducts scans based on these parameters, resulting in the creation of an electric field intensity diagram for the two-dimensional hexagonal photonic crystal, depicted in figure 3. Similarly, the energy band diagram for the same photonic crystal is illustrated in figure 4.

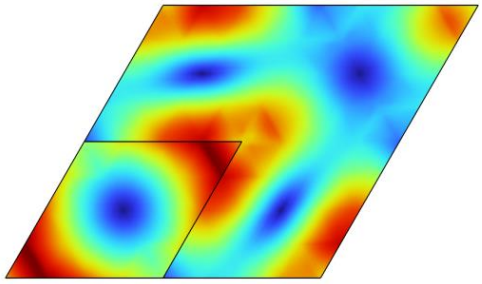


Figure 3. Electric field intensity diagram of two-dimensional hexagonal photonic crystals

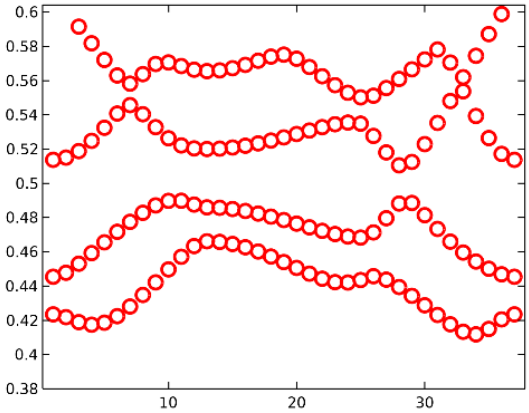


Figure 4. Band diagrams of two-dimensional hexagonal photonic crystals

4. Conclusions

In this study, we utilized the COMSOL software to simulate the band diagram of a two-dimensional hexagonal photonic crystal employing the plane wave expansion method and finite element method. Our results reveal that the electric field intensity notably amplifies at the high symmetry points of the lattice, indicating a higher propensity for electromagnetic wave presence at these locations. Moreover, significant energy gaps between the second and third energy bands were observed, suggesting avenues for further investigation. This narrow bandgap can be seen as a filter that has filtering properties for specific frequency light waves, and can be further studied as a device in the future

Furthermore, we can adjust the material and size of the optical lattice, the type and proportion of doped atoms to further regulate the band structure, especially the band gap. These simulation calculations play an important role in guiding the experiments of optical metamaterials

The intuitive nature of our simulation results underscores their potential for universal application. The user-friendly interface of COMSOL, coupled with its high accuracy, enhances the accessibility of our findings to researchers and practitioners alike.

Looking ahead, our research opens doors to several promising avenues. Firstly, exploring the underlying mechanisms contributing to the observed energy band structures could provide deeper insights into the behavior of electromagnetic waves in photonic crystals. Secondly, investigating novel methods to manipulate and optimize these energy bands could lead to the development of more efficient photonic devices with tailored functionalities. Finally, integrating experimental validations with computational simulations could offer a comprehensive understanding of the practical implications of our findings, paving the way for advancements in photonic crystal technology.

In essence, our study not only sheds light on the fundamental properties of two-dimensional hexagonal photonic crystals but also sets the stage for future explorations aimed at harnessing their full potential in various applications.

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