Seven-hole graphene photonic crystal

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Abstract. This study investigates the spatial electric field and band diagram of 2D photonic crystals using COMSOL simulation. This paper establishes two models to analyze the characteristics of photonic crystals. The first model involves digging seven standard round air columns from hexagonal graphene material and filling a central air column with tin oxide medium. The air columns disrupt the overall periodicity, and the electron wave function in the electric field graph is localized around the six air columns. The second model consists of six standard round tin oxide dielectric columns and a middle standard round graphene dielectric column, separated by air. The overall periodicity is disrupted, and the electron wave function in the electric field graph is localized around the six-tin oxide dielectric columns. This paper finds that disordered impurities in the 2D crystal structure can disrupt the periodicity of the lattice, leading to the localization of the electric field. These discoveries enhance our comprehension of the characteristics of photonic crystals and their possible uses in diverse domains.

Keywords: Photonic crystal, Graphene, Hole, Doped.

1. Introduction

S. John creats photonic crystals in 1987. It is artificial metastructures with periodic modulation of dielectric constants by spatial positions, and have characteristics such as photonic bands and bandgaps. Cheng Qiyun et al. starts from the Helmholtz equation and combines it with the Bloch state to derive the eigen equation of photonic crystals in partial differential form [1]. The attained eigenfrequencies result in the formation of energy bands. The viability of this method is confirmed by comparing the simulation outcomes with traditional calculations. Fangfang employed linear finite element discretization, in conjunction with COMSOL software, to determine the band structure of a 2D honeycomb photonic crystal lattice derived from triangular lattice cells [2]. The research demonstrated that the mathematical model and simulation algorithm for the band structure of the 2D novel honeycomb photonic crystal were accurate and efficient. Amjady employed the plane wave expansion technique to derive the master equations for the transverse magnetic field mode and transverse electric field mode of 2D photonic crystals, leading to the ascertainment of the complete bandgap in both modes [3]. The study of the variation in the width and center frequency position of the complete bandgap of 2D photonic crystals with the filling ratio and background dielectric constant achieved the optimization of the complete photonic bandgap of 2D photonic crystals. Ma Kunlong utilized the plane wave expansion method to derive the eigenequations of TE and TM waves, followed by a Fourier transform [4]. The bandgap structure of 2D functional photonic crystals significantly differs from that of 2D conventional photonic crystals, and the number, position, and width of bandgaps in 2D functional photonic crystals vary with the parameter k, achieving the tunability of the bandgap structure of 2D functional photonic crystals. SHI Biao et al. used the extended DtN mapping method to calculate and validate the rationality of the bandgap structure of 2D piezoelectric photonic crystals in the terahertz frequency band [5]. Reference used the plane wave expansion method and the COMSOL finite element method to calculate and compare the bandgap structures of 2D conventional and functional photonic crystals under the same parameters. The basic funamental of BP neural network [6-10].

2. Photonic crystal theory

The Maxwell equations can be used to describe the propagation of electromagnetic waves in photonic crystals:

$$\begin{cases} \nabla \bullet D = \rho \\ \nabla \bullet B = 0 \\ \nabla \times E + \dfrac{\partial B}{\partial t} = \rho \\ \nabla \times H - \dfrac{\partial}{\partial t} D = J \end{cases} \tag{1}$$

Of these, E and B represent the macroscopic electromagnetic fields and magnetic induction fields, respectively. D is the potential shift vector, while H denotes the magnetic field. ρ and J are the free charge density and current density, respectively.

Due to the non-magnetic nature of photonic crystals, there are

$$B = \mu_0 \mu(r) H \tag{2}$$

$$D = \varepsilon_0 \varepsilon(r) E \tag{3}$$

Of these, μ and ε are the relative magnetic permeability and relative dielectric constant in vacuum, while μ and ε are the absolute magnetic permeability and absolute dielectric constant. Therefore, the Maxwell equations can derive the following wave equations

$$\frac{1}{c^2}\frac{\partial^2 D}{\partial t^2} + \nabla\left(\frac{1}{\mu(r)}\nabla \times \frac{D}{\varepsilon(r)}\right) = 0 \tag{4}$$

Considering the z-direction, equation (2) is

$$\frac{d^2}{dt^2} E(z) + \frac{\omega^2}{c^2}\varepsilon(z) E(z) = 0 \tag{5}$$

Finally, a transcendental equation can be obtained

$$\cos k(d_1 + d_2) = \cos\frac{n_1 \omega d_1}{c}\cos\frac{n_2 \omega d_2}{c} - \frac{1}{2}\left(\frac{n_1}{n_2} + \frac{n_2}{n_1}\right)\sin\frac{n_1 \omega d_1}{c}\sin\frac{n_2 \omega d_2}{c} \tag{6}$$

The dispersion relation for the propagation of electromagnetic waves in a one-dimensional periodic photonic crystal can be found using Equation (6).

Meanwhile, the eigensolutions and dispersion relations for the 1D complete monatomic chain system are as follows:

$$\boldsymbol{u_n = Ae^{i[qnd-\omega(q)t]}, q \in 1BZ} \tag{7}$$

$$\boldsymbol{\omega(q) = \omega_m \left| sin\frac{1}{2}qd \right|, \omega_m = 2\sqrt{\frac{\beta}{M}}} \tag{8}$$

$$\begin{cases} \boldsymbol{q = q_1 + iq_2} \\ \boldsymbol{q_2 \neq 0} \end{cases} \tag{9}$$

Thus can be obtained

$$\frac{\omega}{\omega_m} = sin\frac{1}{2}q_1 darcosh\frac{1}{2}q_2 d + icos\frac{1}{2}q_1 dsinh\frac{1}{2}q_2 d \tag{10}$$

Then

$$\boldsymbol{\frac{1}{2}q_1 d = \left(h \pm \frac{1}{2}\right)\pi} \tag{11}$$

And

$$\boldsymbol{q_1 = \left(h \pm \frac{1}{2}\right)\frac{2\pi}{d} = K_h \pm \frac{\pi}{d}} \tag{12}$$

We can get

$$\boldsymbol{q = \frac{\pi}{d} + i\frac{2}{a}arcosh\frac{\omega}{\omega_m}} \tag{13}$$

$$\boldsymbol{u_n = A(-1)^n e^{-n\alpha} e^{-i\omega t}} \tag{14}$$

WHERE α = 2arcosh (ω/ω_m).

3. Simulation model

A band analysis was performed on 2D hexagonal graphene photonic crystals that were doped with tin oxide. The fundamental parameters of the 2D graphene photonic crystal are the relative dielectric constant of the background medium, graphene, is εc=13, while the tin oxide column has a relative dielectric constant of εa=1. The structural schematic of the 2D graphene doped photonic crystal is displayed in Figure 1. The radius of the tin oxide column is r=0.48nm, with an edge length of a=1nm, which is also the lattice constant.

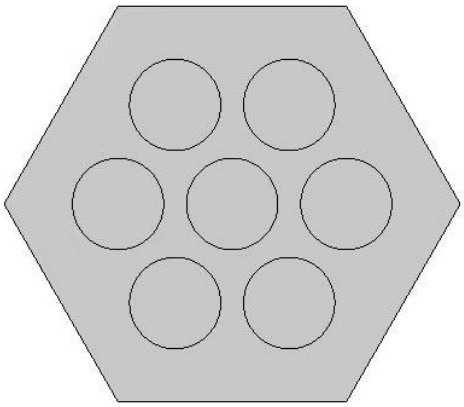


Figure 1. Structure

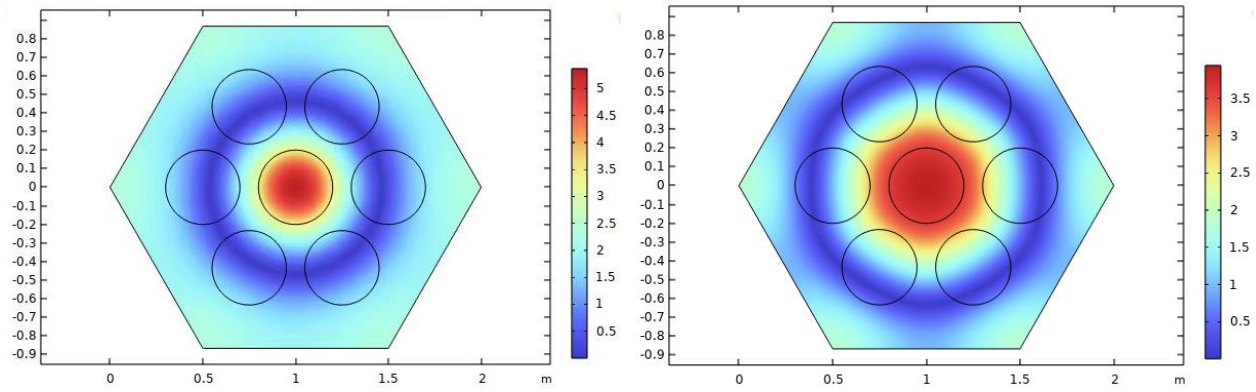


Figure 2. The electric field

The electric field height map of the 2D graphene doped photonic crystal TM mode made is shown in Figure 2. It can be seen that there is a significant local vibration in the electric field near tin oxide.

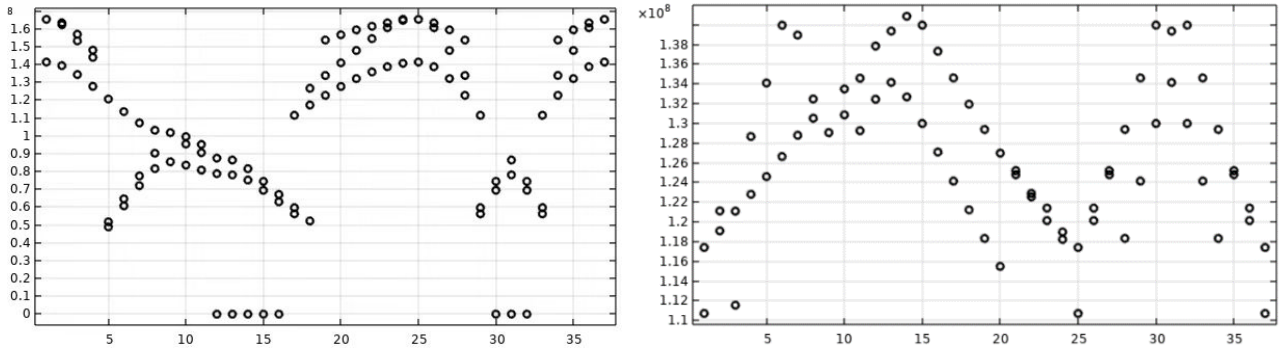


Figure 3. The band structures

The band structure of 2D hexagonal graphene doped photonic crystal TM mode is Figure 3. It can be seen the TM mode of this structure is in f1 = 1.414Hz f2 = 1.513Hz and the bandgap widths are $\Delta\omega 1 = 0.022$Hz and $\Delta\omega 2 = 0.024$Hz.

4. Conclusion

We studied the spatial electric field and band diagram of 2D photonic crystals by use of the comsol simulation. This article establishes two models in the study of photonic crystals. The first model is that we dig seven standard round air columns from the hexagonal Graphene material, and fill tin oxide medium into the most central air column. We study the distribution and band diagrams of the electric field in the COMSOL. The air columns disrupt the overall periodicity. And the electron wave function in the electric field graph is localized around six air columns. The second model is six standard round tin oxide dielectric columns and the middle standard round Graphene dielectric column. Six tin oxides are separated by air, and the overall periodicity is disrupted. The electron wave function in the electric field graph is localized around the six-tin oxide dielectric columns. Six tin oxides are separated by air, and the overall periodicity is disrupted. The electron wave function in the electric field graph is localized around the six-tin oxide dielectric columns. By establishing two models in COMSOL, we obtained spatial electric field and band diagrams, and found that disordered impurities in the 2D crystal structure can disrupt the periodicity of the lattice. And the electron wave function will be localized around the impurities, leading to the localization of the electric field.

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