Differences of Band Gap Characteristics of Square and Triangular Lattice Photonic Crystals in Terahertz Range

Jie Zha, Zhi-Yong Zhong, Huai-Wu Zhang, Qi-Ye Wen, and Yuan-Xun Li

Abstract—Band gap characteristics of the photonic crystals in terahertz range with square lattice and triangular lattice of GaAs cylinders are comparatively studied by means of plane wave method (PWM). The influence of the radius on the band gap width is analyzed and the critical values where the band gap appears are put forward. The results show that the maximum band gap width of photonic crystal with triangular lattice of GaAs cylinders is much wider than that of photonic crystal with square lattice. The research provides a theoretic basis for the development of terahertz (THz) devices.

Index Terms—Band gap structure, critical value, expansion method, photonic crystals, plane wave GaAs, terahertz waves.

1. Introduction

During the last decade, THz wavelength, which is in the spectrum between light wave and microwave, has attracted plenty of interests due to its special uses in medical imaging, space communication, and military applications[1][3]. Some applications of the THz waves require waveform and spectrum manipulation, which can be achieved by employing properly designed photonic crystals (PCs)[4][7]. It is also known as photonic microstructures or photonic band gaps (PBGs) structures which were first mentioned by Yablonovitch[8] and John[9] in 1987. For frequencies within the PBGs, wave propagation is forbidden and many photonic devices have been proposed and designed based on this phenomenon. Recently, considerable attention has been paid on two dimensional (2D) and three dimensional (3D) structures expecting to obtain absolute photonic band gaps common to E and H polarized waves, in analogy to the electronic band gaps in natural semiconductor crystals[10]. In this paper, we first design two types of compound lattice, and perform theoretical simulations utilizing the plane-wave expansion method.

The plane-wave method, which can solve the full-vector wave equation for the magnetic field, as the name implies, is based on a plane-wave expansion of the field and an expansion of the position-dependent dielectric constant. The method has a very general nature for treating periodic structure, and can be applied to solve one-, two-, and three-dimensional problems. It allows one to calculate the photonic band diagrams of photonic crystals, the possible existence, width, and positioning of any PBG. In this paper, we design two types THz photonic crystals of GaAs cylinders, and calculate the band gap with E-propagation wave’s model (using 441 plane waves). At last, the maximum band gap width and the critical value are obtained and some differences between the two types PCs are found.

2. Design of Photonic Crystals

Wave propagation in the photonic crystals can be described by Maxwell equation

\[
\nabla \times \left[ \frac{1}{\varepsilon(x)} \nabla \times E \right] = \frac{\omega^2}{c^2} E \quad (1)
\]

\[
\nabla \times \left[ \frac{1}{\varepsilon(x)} \nabla \times H \right] = \frac{\omega^2}{c^2} H \quad (2)
\]

Taking advantage of the periodic nature of the problem, the dielectric constant can be expressed as a Fourier series expansion:

\[
\varepsilon^{-1}(x) = \sum_{G} K(G) e^{iGx} \quad (3)
\]

where \(\varepsilon^{-1}(x)\) is the position-dependent dielectric constant of the periodic structure. The \(H\)-field can be expanded into a sum of plane waves using Bloch’s theorem as

\[
H_{i}(x, \omega) = \sum_{G} A(K + G) e^{i(K \cdot x - \omega t)} \quad (4)
\]
where \( \mathbf{K} \) is a wave vector in the Brillouin zone, \( \mathbf{G} \) represents a lattice vector in reciprocal space, describing the periodic structure, and \( H(\mathbf{K}+\mathbf{G}) \) is the expansion coefficient corresponding to \( \mathbf{G} \).

We first consider the \( H \)-polarization. \( H \) and \( E \) can be written as

\[
H(x_{11}, t) = H_0(x_{11}, \omega) e^{i \omega t} \quad (5)
\]

\[
E(x_{11}, t) = E_0(x_{11}, \omega) e^{i \omega t} = (E_1(x_{11}, \omega), E_2(x_{11}, \omega), 0) e^{i \omega t}. \quad (6)
\]

By substituting (5) and (6) into (2), we can obtain

\[
\frac{\partial}{\partial x_1} \left( \frac{1}{\varepsilon(x_{11})} \frac{\partial H_1}{\partial x_1} \right) + \frac{\partial}{\partial x_2} \left( \frac{1}{\varepsilon(x_{11})} \frac{\partial H_2}{\partial x_2} \right) = -\frac{\omega^2}{c^2} H_3. \quad (7)
\]

Finally, taking (3) and (4) into (7), we finally get

\[
\sum \mathbf{K} (\mathbf{G}-\mathbf{G}') (\mathbf{k} + \mathbf{G}) \cdot \mathbf{d} (\mathbf{k} + \mathbf{G}') = \frac{\omega^2}{c^2} A(\mathbf{k} + \mathbf{G}). \quad (8)
\]

By the same method, for a single mode and \( E \) polarized waves, we can obtain

\[
\sum \mathbf{K} (\mathbf{G}-\mathbf{G}') (\mathbf{k} + \mathbf{G}') \cdot \mathbf{b} (\mathbf{k} + \mathbf{G}') = \frac{\omega^2}{c^2} B(\mathbf{k} + \mathbf{G}). \quad (9)
\]

In the case of our square and triangular compound lattice with constant \( a \), the unit cell contains two same dielectric cylinders with dielectric constant \( \varepsilon_a \) (background of air) and diameter of \( r \) which are GaAs dielectric cylinders with dielectric constant \( \varepsilon_b \). Now we obtain

\[
\mathbf{K}(\mathbf{G}) = \begin{cases} 
\frac{1}{\varepsilon_a} f \frac{1}{\varepsilon_b} (1-f), & \text{if } \mathbf{G} = \mathbf{0} \\
\frac{1}{\varepsilon_a} f \frac{2 J_1(r |\mathbf{G}|)}{r |\mathbf{G}|} , & \text{if } \mathbf{G} \neq \mathbf{0} 
\end{cases} \quad (10)
\]

where \( J_1 \) is the first order Bessel function, and \( f \) is the filling factor, which can be calculated as follows respectively:

\[
f = \frac{S_r}{S_a} = \frac{\pi r^2}{a^2} \quad \text{(Square lattice)} \quad (11)
\]

\[
f = \frac{S_r}{S_a} = \frac{2 \pi r^2}{\sqrt{3} a^2} \quad \text{(Triangular lattice). \quad (12)}
\]

With (10), we can solve (8) and (9) by the standard matrix digitalization method and perform numerical calculations.

3. Results and Discussion

3.1 Physical Model

\( \varepsilon_a \) and \( \varepsilon_b \) are set to be 1 (the dielectric constant for air) and 11.6 (the dielectric constant for GaAs), lattice constant \( a \) is set to be \( 10^{-6} \) m. Fig. 1 illustrates the cylinder constitutes of square and triangular lattice. Fig. 1 shows the two lattices models and the relative Brillouin region.

3.2 Calculation of Band Gaps

Fig. 2 shows the maximum photonic band gap varied with \( r/a \). As seen from Fig. 2, \( r/a \) is a key factor which affects the PBGs in the square lattice and the triangular lattice microstructure THz PCs. In the range of 0 Hz to 1.8 THz, when the radius of GaAs cylinders is changed from 0.06 to 0.45, it can be found that only when \( 0.08 \leq r/a \leq 0.43 \), the band gap of 2D square lattice will appear, while in the case of triangular lattice PCs, the band gap will appear when \( 0.06 \leq r/a \leq 0.45 \). So the critical values and the radius of triangular lattice PCs are higher than that of square lattice PCs. When \( r/a = 0.17 \) (square lattice) and \( r/a = 0.15 \) (triangular lattice), the maximum band gap could be obtained respectively.

Fig. 3 is an example of three band gaps of square lattice and Fig. 4 is for triangular lattice. From the simulation results, it is found that with the variety of \( r/a \) there is no more than three band gaps. By introducing the different photonic band gaps, some different THz waveguide devices can be obtain.
Fig. 3. Three band gaps of square lattice \((r/a=0.3)\).

Fig. 4. Three band gaps of triangular lattice \((r/a=0.24)\).

Fig. 5. Maximum band gap of square lattice \((r/a=0.17)\).

Fig. 6. Maximum band gap of triangular lattice \((r/a=0.15)\).

3.3 Effect of Dielectric Constant

When the dielectric constant \(\varepsilon_b\) is changed, it can be found that the centre frequency of the maximum band gap is shifted down, and the maximum band gap width is increased. Table 1 shows the results. It can be seen the two PCs present the same rule.

<table>
<thead>
<tr>
<th>Item</th>
<th>Square lattice</th>
<th>Triangular lattice</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\varepsilon_b)</td>
<td>(f_c) (THz)</td>
<td>(W) (THz)</td>
</tr>
<tr>
<td>11.6</td>
<td>0.3842</td>
<td>0.1396</td>
</tr>
<tr>
<td>13.6</td>
<td>0.3789</td>
<td>0.1517</td>
</tr>
<tr>
<td>15.6</td>
<td>0.3766</td>
<td>0.1620</td>
</tr>
</tbody>
</table>

4. Conclusion

We present the photonic crystal of two types of compound lattices and obtain the band gaps of the two types of PBGs for THz. Through a great deal of calculation and analysis, we observe that the radius of the dielectric cylinder can significantly affect the band gap in THz range and exhibit a regular change. It is proved that the band gap only appear between the critical values, and the maximum band gap of triangular lattice PCs is higher than that of square lattice PCs. Our work is helpful to the design of devices of photonic crystals in THz range such as filters, reflectors, and switches.

References

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