Analysis of Photonic-Band Dispersion Characteristics in Photonic Crystal Consisting of Periodic Atoms for Nano-meter Waveguides

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Abstract Nano-meter wave waveguide is a basic element of Nano-meter wave devices, which will be important in nano-technologies, bio-engineering, cell membrane, genetics, and so on. Until now, the nano-meter wave waveguide characteristics have hardly been examined and effective nano-meter wave waveguides have not been developed. We have investigated photonic crystal with a lattice constant of the same order as the wavelength of nano-meter waves.

In the nano-meter wave region, the refractive index of a material becomes smaller than 1, and it has the characteristics depending on the incident electromagnetic wave. We have calculated photonic band structures for two-dimensional C and Mo arrays with plane wave expansion method. Although complete bandgaps in these matters do not exist, we have found the existence of local bandgaps.

Keywords: photonic crystal, nano-meter wave, photonic bandgap, plane wave expansion method

1. Introduction

Photonic crystal waveguides have been attracting attention in optical wavelength region\(^{(1)-(3)}\). The photonic crystal consists of periodic dielectric medium of the order of the optical wavelength, which is used to guide waves with the cladding of the photonic crystal. The periodic structure is artificially made in optical wavelength region. For the nano-meter waves, however, natural atomic array structure is regarded as the periodic structure for the photonic crystal\(^{(4)-(7)}\). The authors have studied fundamental characteristics of nano-meter waveguides\(^{(8)-(11)}\). The waveguides for nano-meter waves will be important fundamental elements for measurements, information transmission and processing in the fields of nano-space condensed matter, bio-engineering, nano-meter devices, cell membrane, and genetics.

For nano-meter waves with the wavelength less than 0.5nm, atomic interval of the medium is the same order as the wavelength, and the material is considered as in a discrete structure. For the wavelength larger than 1nm, a periodic structure of molecules is effective. To study nano-meter waveguides in detail, we have to investigate electromagnetic wave propagation in periodic structures. The authors discussed quantum mechanically a micro refractive-index distribution in an electron distribution field of an atom\(^{(12)}\). Also, scattering and near-field characteristics of electromagnetic waves were studied in a discrete atomic array\(^{(10)-(13)}\). Based on these studies, bandgap characteristics of nano-meter waves in periodic structures are discussed as a fundamental research for realizing waveguides for nano-meter waves in this paper.

We discuss photonic bandgaps, where wave propagation is prohibited in photonic crystal consisting of periodic array of two kinds of dielectrics with the lattice constant is of the order of the electromagnetic wavelength. In the nano-meter wave region, the atomic lattice constant is the same order of the wavelength, and the natural crystal will be used as the photonic crystals.

Various numerical methods have been used to analyze the frequency dispersion characteristics and optical characteristics in photonic crystals. The plane wave expansion method is used in general\(^{(12)-(13)}\). For photonic crystals with a large difference in the dielectric constants, other methods such as the transfer matrix method, the Körning-Kohn-Rostoker (KKR) method, and FDTD method have been employed. The FDTD method has been used to evaluate the optical characteristics in slab-type two-dimensional crystal with defects in the periodic array. In this paper, we analyze the photonic band structure in nano-meter wave region using the plane wave expansion method.

2. Nano-meter Electromagnetic Waves in Periodic Structure Medium

We consider crystal structure with the position vector of the atomic nucleus \( \mathbf{R}_{\nu},(\nu) \), and periodic length in the \( x \), \( y \) and \( z \) direction, \( d_x \), \( d_y \) and \( d_z \) respectively.

In crystal matter having periodic atom structure as shown in Fig.1, the refractive index is given by

\[
n(R_x) = \frac{\rho(R_x, R_{\nu}, \lambda)}{m_0^2 \varepsilon_s (1 - j\gamma / m_0)} \frac{\varepsilon_0^2}{(1 - j\gamma / m_0)} \left[ 1 - \frac{\rho(R_x, R_{\nu}, \lambda)}{m_0^2 \varepsilon_s (1 - j\gamma / m_0)} \right]^{1/2}
\]

From Eq.(2), the refractive index is obtained as

\[
n = 1 - \delta - j\eta \equiv n - j\eta
\]

\[
\delta = \frac{\rho c}{2\pi} f_1, \quad \eta = \frac{\rho c}{2\pi} f_2
\]

where \( c_0 \) is the classical radius of electron, \( \lambda \) is the wavelength of the nano-meter wave, \( f_1 \) and \( f_2 \) are scattering factors. The

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absorption is written as \( \eta \propto \lambda^2 \lambda^{-1} \) and each atom has its natural absorption field.

In the nano-meter wave region, the refractive index decreases and the absorption increases as the wavelength increases. This dispersion is complicated in the wavelength larger than 10nm due to the natural absorption characteristics. The real part of the refractive index in the wavelength less than 1mm is larger than \( n_\infty \approx 0.995 \) in most atoms. \(^{(14)}\) In the calculation of photonic crystal, we use the refractive indices measured by Henke \(^{(14)}\) as the circular cylinder, instead of the use of Eq.(2).

We consider two-dimensional problem to show the fundamental physical characteristics. Two-dimensional lattice is defined by the two primitive translation vectors, \( \mathbf{a}_1 \) and \( \mathbf{a}_2 \), which correspond to \( \mathbf{d}_y \) and \( \mathbf{d}_z \) respectively. The atomic array at \( \mathbf{r} \) is regarded as the same as that at \( \mathbf{r} + \mathbf{r}_l \)

\[
(3) \quad \mathbf{r} = \mathbf{r}_l + l_1 \mathbf{a}_1 + l_2 \mathbf{a}_2
\]

where \( l_1 \) and \( l_2 \) are arbitrary integers.

Two-dimensional Bravais lattice is given by

\[
(4) \quad \mathbf{r}(l) = l_1 \mathbf{a}_1 + l_2 \mathbf{a}_2
\]

The area of the unit cell is equal to that of Wigner-Seitz cell and is given by \( a^2 = |\mathbf{a}_1 \times \mathbf{a}_2| \). The primitive translation vectors in the reciprocal lattice \( \mathbf{b}_1 \) and \( \mathbf{b}_2 \) are defined by

\[
(5) \quad \mathbf{b}_1 = \frac{2\pi}{a_1} (1,0,-a_2)
\]

\[
(6) \quad \mathbf{b}_2 = \frac{2\pi}{a_2} (0,1,a_1)
\]

\[
(7) \quad \mathbf{b}_i \cdot \mathbf{a}_j = 2\pi\delta_{ij}
\]

where \( a^2_j \) is the j-direction component of \( \mathbf{a}_j \).

The position of the reciprocal lattice is given by the reciprocal lattice vector

\[
G(h) = h_1 \mathbf{b}_1 + h_2 \mathbf{b}_2
\]

where \( h_1 \) and \( h_2 \) are integers. The Brillouin zone is defined as the Wigner-Seitz cell in the reciprocal lattice.

3. Photonic Band Structure in Nano-meter Wave Region

We describe the photonic band structure consisting of periodic matter of \( \varepsilon(r) \) using the plane wave expansion method.

3.1 In Case of TM Wave

We consider the TM wave in two-dimensional periodic structure given by

\[
(9) \quad \begin{align*}
H(r,t) &= (H_x(y,z) | \omega, 0,0) \exp(-j\omega t) \\
E_r(r,t) &= (0, E_r(y,z) | \omega, 0,0) \exp(-j\omega t)
\end{align*}
\]

From Maxwell equations, we obtain the wave equation for \( H_x \)

\[
(10) \quad \frac{\partial^2}{\partial y^2} \left( \frac{1}{\varepsilon(r)} \frac{\partial H_x}{\partial y} \right) + \frac{\partial^2}{\partial z^2} \left( \frac{1}{\varepsilon(r)} \frac{\partial H_z}{\partial z} \right) = -\frac{\omega^2}{c^2} H_x
\]

where \( c^2 = 1/\varepsilon_0 \mu_0 \).

We expand \( 1/\varepsilon(r) \) and \( H_x \) as

\[
(11) \quad \frac{1}{\varepsilon(r)} = \sum_G \hat{\varepsilon}(G)e^{jG \cdot r}
\]

\[
(12) \quad H_x(r|\omega) = \sum_G A(k|G)e^{j(k \cdot r + G \cdot r)}
\]

where \( k = k_x i \mathbf{a}_1 + k_y i \mathbf{a}_2 \), \( \mathbf{G} \) is the reciprocal lattice vector as given in Eq.(8). From Eq.(10), we have

\[
(13) \quad \sum_G (k + G \cdot i \mathbf{a}_1 + G \cdot i \mathbf{a}_2) \cdot \hat{\varepsilon}(G) \cdot (G - G) \cdot A(k|G) = \frac{\omega^2}{c^2} A(k|G)
\]

The summation about \( G \) means the summation regarding infinite reciprocal lattice vector. Here, we approximately calculate this summation using 271 reciprocal lattice vectors, \( G_1, G_2, \ldots, G_{271} \).

When the \( G \) is substituted by \( G_1, G_2, \ldots, G_{271} \), we obtain the following matrix form

\[
M \mathbf{X} + \omega^2 \mathbf{C} \mathbf{X} = \omega^2 \mathbf{K} \mathbf{X}
\]

\[
M = \sum_{G} \langle k + G | \hat{\varepsilon}(G) | G \rangle
\]

\[
K = \sum_{G} \langle k + G | \hat{\varepsilon}(G - G) | G \rangle
\]

\[
C = \sum_{G} \langle k + G | \hat{\varepsilon}(G) | G \rangle
\]

This equation is the eigen value problem for general symmetric matrix, and is easily solved.

3.2 In Case of TE Wave

Next, we consider TE wave in two-dimensional periodic structure which is uniform in the x direction.

\[
(15) \quad \begin{align*}
H(r,t) &= (H_y(y,z) | \omega, 0,0) \exp(-j\omega t) \\
E_z(r,t) &= (0, E_z(y,z) | \omega, 0,0) \exp(-j\omega t)
\end{align*}
\]

From Maxwell equations, we have

\[
(16) \quad \frac{\partial^2}{\partial y^2} \left( \frac{1}{\varepsilon(r)} \frac{\partial E_z}{\partial y} \right) + \frac{\partial^2}{\partial z^2} \left( \frac{1}{\varepsilon(r)} \frac{\partial E_z}{\partial z} \right) = -\frac{\omega^2}{c^2} E_z
\]

By expanding \( 1/\varepsilon(r) \) and \( E_z \) as in the similar manner for TE wave, we have
\[
\frac{1}{\varepsilon_a r} = \sum \frac{k(G)e^{iGr}}{G} \quad \text{........................................(17)}
\]

\[
E_\gamma r |\alpha \rangle = \sum B(k|G)e^{i(k-G)r} \quad \text{........................................(18)}
\]

We obtain the following equation in a similar manner as in TM wave
\[
\sum_{k} (k + G) \cdot (k + G') \hat{k'(G-G')} B(k|G) = \frac{\omega^2}{c^2} B(k|G)
\]
\text{........................................(19)}

This is asymmetric eigen value problem. By defining C by
\[
C(k|G) = (k + G) B(k|G)
\]

we have
\[
\sum_{k} (k + G) \hat{k'(k+G')k+G} C(k|G) = \frac{\omega^2}{c^2} C(k|G) \quad \text{........................................(20)}
\]

Using 271 reciprocal lattice vectors, this can be translated to the symmetric eigen value problem as

\[
\begin{pmatrix}
MX = \frac{\omega^2}{c^2} X \\
M_{\gamma} = (k + G_i) \cdot (k + G_j) \hat{k'(G_i-G_j)} \\
X = \begin{pmatrix}
C(k|G_i) \\
M \\
C(k|G_j)
\end{pmatrix}
\end{pmatrix}
\quad \text{........................................(21)}
\]

To find \( \hat{k'(G)} \), we write

\[
\frac{1}{\varepsilon_a r} = \frac{1}{\varepsilon_s} + \frac{1}{\varepsilon_s} \sum S(r - r(l))
\]

\[
S(r) = \begin{cases} 
1 & r \in R \\
0 & r \notin R
\end{cases}
\quad \text{........................................(22)}
\]

where \( R \) is the cross section of the matter, \( \varepsilon_s \) is the relative dielectric constant, \( \varepsilon_a \) is that of the background.

The Fourier coefficient \( \hat{k'(G)} \) is given by

\[
\frac{1}{a_s^2} \int d^2r e^{-iGr} \frac{1}{\varepsilon(r)} \int \frac{1}{\varepsilon_s} + \frac{1}{\varepsilon_s} \sum S(r - r(l))
\]

\[
\hat{k'(G)} = \begin{pmatrix}
\frac{1}{\varepsilon_s} | f + \frac{1}{\varepsilon_s}(1 - f) & \text{if } G = 0 \\
\frac{1}{\varepsilon_s} \frac{1}{\varepsilon_s} \int d^2r e^{-iGr} & \text{if } G \neq 0
\end{pmatrix}
\quad \text{........................................(24)}
\]

where \( f \) is the occupation factor and is \( f = d_0/a_0 \), and \( a_0 \) is the area of \( R \). When the matter is the circle of radius \( R \),

\[
J_1(x) = \text{Bessel function.}
\]

\[\text{The photonic band characteristics can be calculated with Eqs.(14) and (21) for TM wave and TE wave, respectively.}
\]

4. Photonic Band Characteristics of Matter for Nano-meter Wave

4.1 Photonic Band Structure of Molybdenum Matter

The periodic structure of molybdenum atom is shown in Fig.2, where the atomic radius \( R = 0.136 \text{nm} \), and the relative dielectric constant of circular cylinder is 0.999503 and the interval between atoms \( a = d_0 = d_1 = 0.314 \text{nm} \). The primitive translation vectors are

\[
a_1 = (a,0) \quad \text{........................................(26)}
\]

\[
a_2 = (0,a) \quad \text{........................................(27)}
\]

The primitive translation vectors in the reciprocal lattice are

\[
b_1 = \frac{2\pi}{a} (1,0) \quad \text{........................................(28)}
\]

\[
b_2 = \frac{2\pi}{a} (0,1) \quad \text{........................................(29)}
\]

The circular cylinder of molybdenum is assumed to exist infinitely periodically in the \( y \) and \( z \) directions.

The calculated frequency dispersion characteristics are shown in Figs.3 ~ 5. The frequency in the vertical axis is normalized by \( a^2/2\pi \). The wave number vector \( k \) varies its direction from \( M, \Gamma \) to \( X \) and return to \( M \) in the irreducible Brillouin zone as shown in the inset figure. The directions \( M \) and \( X \) correspond to \( (\hat{k}_x + \hat{k}_y) / \sqrt{2} \) and \( \hat{k}_z \), respectively. For TM wave, two band gaps exist between \( M \) and \( \Gamma \) and between \( \Gamma \) and \( X \), although the frequencies of these band gaps are different.

4.2 Photonic Band Structure of Carbon Matter

We consider the dielectric circular cylinder model of carbon in hexagonal lattice structure as shown in Fig.6. The atomic radius is \( R = 0.077 \text{nm} \), and the atomic interval is \( a = 0.142 \text{nm} \). The relative dielectric constant of the cylinder is assumed to be 0.999896. The primitive translation vectors are

\[
a_i = \left( \sqrt{3} a_0, \frac{1}{2} a, 0 \right) \quad \text{........................................(30)}
\]

Fig. 2. Periodic structure of Mo atom

\[
a = d_0 = d_1 = 3.14 \text{Å}
\]
Fig. 3. Band structure of Mo atom

Fig. 4. Detailed band structure of Mo atom (around M)

Fig. 5. Detailed band structure of Mo atom (around X)

\[ a_x = \left( \frac{\sqrt{3}}{2}, a_x = \frac{1}{2} \right) \]  

The primitive translation vectors in the reciprocal lattice are

\[ b_x = \frac{2\pi}{a_x} \left( 1, a_x = \frac{1}{2} \right) \]  \( a_x = a_x \times a_x \)

\[ b_x = \frac{2\pi}{a_x} \left( \frac{\sqrt{3}}{2}, a_x = \frac{1}{2} \right) \]  \( a_x = a_x \times a_x \)

where \( a_x = a_x \times a_x \).

Fig. 6. Periodic structure of C atom

Fig. 7. Band structure of C atom

Fig. 8. Detailed band structure of C atom (around X)

Fig. 9. Detailed band structure of C atom (around K)

The frequency dispersion characteristics for TM and TE waves are shown in Figs. 7 – 9. There are two bandgaps between M and \( \Gamma \) and between \( \Gamma \) and K for TM wave, although the frequencies
are different. The directions $\mathbf{K}$ and $\mathbf{M}$ correspond to $(k_y + 2k_x)/\sqrt{3}$ and $k_x$, respectively. For TE wave, a bandgap is found between $\Gamma$ and $K$.

5. Conclusions

Photonic bandgap structures and the dispersion characteristics are investigated for two-dimensional periodic atomic structures in the region of nano-meter wave using the plane wave expansion method. Although complete bandgap was not found for molybdenum and carbon matters, local bandgaps are found for both matters. For molybdenum the bandgaps are between $\Gamma$ and $X$ for TE wave and between $M$ and $\Gamma$ and $X$ for TM wave. For carbon crystal, the bandgaps are between $M$ and $\Gamma$ and between $\Gamma$ and $K$ for TE wave and between $\Gamma$ and $K$ for TM wave. The bandwidth for these bandgaps are of the order of THz. The two-dimensional model discussed in this paper do not simulate the real periodic atoms, though fundamental characteristics of bandgap in nano-meter wave region were found. Detail analysis with three-dimensional atom models is indispensable to realize waveguides consisting of photonic crystal of atoms, and will be studied in future. We will continue to study to find atomic structures having complete bandgap in the nano-meter wave region for realizing effective waveguide structures.

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