Guided mode extraction in monolayer colloidal crystals based on the phase variation of reflection and transmission coefficients

Seyed Amir Hossein Nekuee *, Mahmood Akbari, Amin Khavasi

Department of Electrical Engineering, Sharif University of Technology, Azadi Avenue, Tehran, Iran

**A R T I C L E   I N F O**

Article history:
Received 28 July 2015
Received in revised form 20 October 2015
Accepted 10 November 2015

**M S C :**
00-01
99-00

**Keywords:**
Guided mode
Colloidal crystal
Band structure

**A B S T R A C T**

An accurate and fast method for guided modes extraction in monolayer colloidal crystals and their inverse replicas is presented. These three-dimensional structures are composed of a monolayer of spherical particles that can easily and simply be prepared by self-assembly method in close packed hexagonal lattices. In this work, we describe how the guided modes, even or odd modes and light cone boundary can be easily determined using phase variations of reflection and transmission coefficients. These coefficients are quickly calculated by Fourier modal method. The band structures are obtained for a monolayer of polystyrene particles and two-dimensional TiO2 inverse opal by this proposed method.

© 2015 Elsevier B.V. All rights reserved.

1. Introduction

Controlling the light propagation is possible by periodic modulation of refractive index in structures that their lattice constants are comparable to light wavelengths. Photonic crystals are structures capable of manipulating the flow of light by a property known as photonic band gaps.

Colloidal crystals are periodic arrays of monodisperse colloidal particles, and can be considered as a class of photonic crystals. They can be prepared in self-assembly approaches, in an easier manner and with lower costs compared to photonic crystal fabrication methods, including optical lithography and etching techniques [1,2].

Two-dimensional or three-dimensional periodic colloidal crystals attract great interest due to these challenges in the fabrication of nanoscale photonic crystals. They can find applications in many areas like bio and chemical sensing [3], solar cells [4], display, templates for fabrication of other materials, and miniature diagnostic systems [5]. Also, much progress has been achieved in fabrication of colloidal crystals with point, line and planar defect in recent years [6,7].

Two-dimensional colloidal crystals are monolayer arrays of monodisperse colloidal microspheres or nanospheres which are prepared mostly and commonly in hexagonal close-packed patterns by different self-assembly methods such as drop coating, dip-coating, spin-coating, electrophoretic deposition and self-assembly at the gas–liquid interface [8]. Non-close-packed and binary colloidal crystals are other types of two-dimensional colloidal crystals. Monolayer inverse opals as well as two-dimensional periodic arrays of nanobowls, nanocaps and hollow spheres are samples of inverse replicas of monolayer colloidal crystals which have been fabricated recently [9].

The confinement of guided modes in monolayer colloidal crystals and their inverse replicas depend on the refractive index of the dielectric spheres and the substrate which they rest on it. High refractive index contrast in these structures lead to three-dimensional confinement of light similar to the photonic crystal slabs which is acquired by two-dimensional band gaps in the plane of periodicity and total internal reflection in the vertical direction [10,11]. Therefore, these colloidal structures can be used in couplers, wavelength filters and optical interconnects as well as optical sensors. Determining waveguide modes of these colloidal structures are very important in design and optimization of these optical devices.

Extracting the waveguide modes of multilayered structures can be done by solving an eigenvalue equation. Both guided and leaky modes in lossless or lossy structures can be found as solutions of the eigenvalue equation [12]. Reflection pole method is another approach that is used for the determination of mode propagation constants in lossless and lossy planar structures [13]. This approach uses the simple principle that modes are the poles of reflection or transmission coefficients of a multilayered system. The
modes and light confinement in monolayer colloidal crystals is studied by full numerical methods, like finite-difference time-domain (FDTD) which are time-consuming [14].

Here we propose a method to determine guided modes of a monolayer of colloidal particles and its inverse replica by following the phase variations of reflection and transmission coefficients. These index-guided modes are poles of reflection and transmission coefficients [13] and based on the Bode diagram theory we demonstrate that these index-guided modes can be obtained efficiently and precisely from phase variations equal to π of (0,0)th reflected and transmitted order. The reflection and transmission coefficients of different diffracted orders are calculated by Fourier Modal Method (FMM). Also, we will show how to distinguish even and odd modes, and how the lower boundary of light cone is determined in the proposed method. The obtained modes form the band structures of these slabs.

This paper is organized as follows. In Section 2 the brief review about FMM implementation is presented. Then, guided mode extraction from reflection and transmission coefficients is described with more details in Section 3. Band structures are obtained for two different structures in Section 4. Finally, the conclusions of this work are summarized in Section 5.

2. FMM implementation

An efficient and accurate calculation method of reflection and transmission coefficients and their subsequent phase is necessary for guided mode extraction in this approach.

In most of two-dimensional colloidal crystals, there is a hexagonal close packed of dielectric spheres between two homogeneous regions. These structures could be analyzed by various numerical methods like rigorous couple wave analysis (RCWA) [15]. Fourier modal method (FMM) is the popular modal method for the analysis of crossed gratings, with simple implementation [16]. Its convergence rate is improved relative to RCWA by applying appropriate factorization rules. In this section only required formulation and necessary details for easy implementation of FMM in 2D colloidal crystals are introduced.

A monolayer of colloidal crystals is two-dimensionally periodic as shown in Fig. 1. As mentioned above gratings that are uniform in vertical direction could be analyzed by FMM. Consequently, using staircase approximation a monolayer of colloidal crystals is divided into 2l+1 sublayers in the z direction. These sublayers of the 2D colloidal crystal are hexagonal lattices of cylindrical rods with various radiuses so that the radius of the middle sublayer is equal to the radius of spherical particles, i.e. R.

Due to the symmetry of a sphere in z direction, it is sufficient that only in l+1 regions of 2l+1 sublayer, the main eigenvalue equation of FMM, i.e.

$$\begin{vmatrix}
F & - (k_0 k_z \cos \delta)^2 & E_1 \\
E_2 & - E_1 & 0
\end{vmatrix} = 0.
$$

is solved where $F$ and $G$ are two square matrices [16]. This eigenvalue problem is acquired in a general nonrectangular coordinate system $(x_1, x_2, x_3)$ which the $x_1$ and $x_2$ axes are parallel to the $x$ and $z$ axes and the angle $\delta$ is between the $x_2$ axis and $y$ axis. Blocks of these significant matrices are made by applying Fourier factorization rules, i.e. Laurent’s and inverse rules to the Fourier series coefficients of permittivity distribution $\epsilon(x_1, x_2)$ in each sublayer. Note that the calculations of Fourier series coefficients and the angle $\delta$ depend on the type of selected unit cell. In this equation $k_0$ is $2\pi / \lambda$ where $\lambda$ is the vacuum wavelength and the mediums are assumed to be nonmagnetic ($\mu = 1$). Also, $k_z$’s are propagation constants of different orders in the $z$ direction and selected such that

$$\text{Re}[k_z] + \text{Im}[k_z] \geq 0$$ (2)

Electric eigenvectors in $x_1$ and $x_2$ directions are denoted by $E_1$ and $E_2$, respectively. Magnetic eigenvectors are obtained by

$$\begin{pmatrix}
H_1 \\
H_2
\end{pmatrix} = \frac{\sec \delta}{k_0 k_z} \begin{pmatrix} E_1 \\ E_2 \end{pmatrix}. \tag{3}
$$

The obtained eigenvectors and eigenvalues in each sublayer of 2D colloidal crystal form the matrices $W_1$, $W_2$ and $\phi$ which are used in the S-matrix algorithm [17]. These matrices can be written as

$$W_1 = \begin{pmatrix} E_{1mn} \\ E_{2mn} \end{pmatrix}, \quad W_2 = \begin{pmatrix} H_{1mn} \\ H_{2mn} \end{pmatrix} \tag{4}
$$

where $h = 2R(2l + 1)$ demonstrate the thickness of each sublayer. Note that S-matrix algorithm is used to match boundary conditions at the interfaces between $2l+1$ sublayers and top and bottom homogeneous regions [17].

The electric and magnetic eigenvectors in homogeneous regions, i.e. bottom and top mediums of spherical particles are calculated just by Rayleigh expansion without the need to solve eigenvalue problem. The main matrices for S-matrix algorithm in the $p$th region are [18]

$$W_1 = I, \quad W_2 = \begin{pmatrix} F^p - A^p \\ B^p - F^p \end{pmatrix} \tag{5}
$$

where $A^p$, $B^p$ and $F^p$ have diagonal elements as

$$A^p_{mn} = \sec \delta \frac{k_0^2 k_{p,z} - k_{s,m}^2}{k_0 k_{s,m}^2},$$

$$B^p_{mn} = \sec \delta \frac{k_0^2 k_{p,z} - k_{s,n}^2}{k_0 k_{s,n}^2},$$

$$F^p_{mn} = \sec \delta \frac{k_0^2 k_{p,z} \sin(\delta) - k_{s,m} k_{s,n}}{k_0 k_{s,m} k_{s,n}} \tag{6}
$$
In the above, $k_{x,m}$ and $k_{z,n}$ are the wave vector of the $(m,n)$th layer. The matrices in Eq. (5) for homogeneous media are the same as those in Eq. (4) for $2l+1$ sublayers in this algorithm, the final $S$-matrix is obtained [17]. Finally, the upward and downward waves in top and bottom homogeneous media relate to each other in this way:

$$
\begin{bmatrix}
    u^d \\
    d^d
\end{bmatrix} = S \begin{bmatrix}
    u^b \\
    d^b
\end{bmatrix} = \begin{bmatrix}
    T_{uu} & R_{ud}^T \\
    R_{du} & T_{dd}
\end{bmatrix} \begin{bmatrix}
    u^b \\
    d^b
\end{bmatrix}
$$

(7)

In the case that the incident plane wave illuminates the structure from the top media ($u^b = 0$ and $d^b \neq 0$) the transmitted $T_{ad}^T$ and reflected $R_{ad}$ coefficients in top and bottom regions can be obtained by Eq. (7).

3. Guided mode extraction

In this section, detecting guided modes, light cone boundary and distinguishing even and odd modes by the phase variations for a monolayer of colloidal crystals in a hexagonal close packed lattice, will be explained.

Guided modes which are poles of reflection and transmission coefficients are detectable by monitoring the phase of reflection and transmission coefficients. This approach is introduced with details in [13] as Reflection Pole Method (RPM). Consider the multilayer structure that is shown in Fig. 2. For TE, propagating modes, the electric field distribution in $y$ direction in the $j$th layer can be written as:

$$
\begin{align*}
E_y &= \hat{y}E_{xy} \exp \left[-i(n_0 - k_z)z \right] \\
E_{xy} &= u_j \exp \left[i k_{xy}(x - x_{j-1}) \right] + d_j \exp \left[-i k_{xy}(x - x_{j-1}) \right]
\end{align*}
$$

(8)

where $k_z = \beta + i n$ is the complex propagation constant. By the amplitudes of the downward ($d_j$) and upward ($u_j$) waves in the $j$th layer the envelop $E_{xy}$ in Eq. (8) is expressed as

$$
E_{xy} = u_j \exp \left[i k_{xy}(x - x_{j-1}) \right] + d_j \exp \left[-i k_{xy}(x - x_{j-1}) \right]
$$

(9)

where $k_{xy} = \sqrt{k_{xy}^2 - k_z^2}$ and $x_{j-1}$ is the boundary between the $j$th and $(j-1)$th layer. By matching the boundary conditions of tangential electric and magnetic field at the interface of adjacent layers and using transfer-matrix analysis the total transfer matrix with the elements $T_{ad}$ [13] is obtained that relates the downward and upward waves at the cover and substrate in the following way:

$$
\begin{align*}
\begin{bmatrix}
    u_c \\
    d_c
\end{bmatrix} &= \begin{bmatrix}
    T_{u1} & T_{u2} \\
    T_{d1} & T_{d2}
\end{bmatrix} \begin{bmatrix}
    u_s \\
    d_s
\end{bmatrix}
\end{align*}
$$

(10)

Therefore, in this multilayer structure the complex reflection and transmission coefficients are derived as:

$$
R_s = \frac{T_{s1}}{T_{s2}}, \quad T_c = \frac{T_{c1}T_{c2} - T_{c1}T_{c3}}{T_{c2}}, \quad R_c = \frac{T_{c2}}{T_{c2}}, \quad T_s = \frac{1}{T_{s2}}
$$

(11)

where $R_s$ and $T_c$ demonstrate the global reflection and transmission from substrate and cover, respectively for the case of a plane wave incident from the substrate. Also, $R_c$ and $T_s$ are defined in a similar way in the case of cover incidence.

The propagation constants of modes ($k_z$) in this multilayer structure are solutions of $T_{s2} = 0$ [19]. In other words, $k_z$'s are the poles of the global coefficients ($R_s$, $T_c$, $R_c$, $T_s$) and make these coefficients infinite. Therefore, the reflection $R$ (or transmission $T$) can be represented as a rational function with poles ($k_z$) and zeros ($\beta$) as:

$$
R(\beta) = A(\beta) \prod_{i=1}^{N_{fp}} \frac{\prod_{p=1}^{M_p} (\beta - k_{z,p})}{\prod_{p=1}^{M_p} (\beta - k_{s,p})}
$$

(12)

where $A(\beta)$ is a slowly varying envelop and $M_s$ and $M_p$ are the number of zeros and poles, respectively. According to Bode-diagram theory [20] it is evident from Eq. (12) that in the location of pure real poles the phase of reflection and transmission varies in the form of a step function with the height $\pi$. Pure real poles represent the guided modes of the structure.

For complex multilayer structures like two-dimensional colloidal crystals it is impossible to find the total reflection and transmission analytically and we should monitor the phase of reflection and transmission coefficients of these structures to determine guided modes. In this paper these characteristic coefficients, as a function of normalized frequency and for a given incident wave vector, are obtained for all diffracted orders by FMM.

A monolayer of polystyrene particles with a refractive index of 1.6 [21] which is fabricated by self-assembly and is suspended in air is considered as the first example. At first $k_x = 2\pi/\lambda$ and $k_y = -k_z/\sqrt{3}$ are considered as a sample for incident wave vectors and reflection and transmission coefficients are obtained. We found that for $(0, 0)$ th diffracted order, there is $f_0$'s that at these points phase variations equal to $\pi$ are found in both $x$ and $y$ components of reflection and transmission coefficients. These phase changes of $(0,0)$th diffracted order are demonstrated for $x$ and $y$ components in Fig. 3(a) and (b), respectively. It is obvious that $f_c = 0.2090$ and $f_s = 0.2206$ are two index-guided modes for these incident propagation constants.

As seen in this figure the phase of reflection and transmission coefficients of $(0,0)$th diffracted order is constant for most of normalized frequencies and changes like a step function with height $\pi$ at certain points. This manner is seen in all diffracted orders, but the points with $\pi$ phase variation may be different for various diffracted orders. Normalized frequencies are considered as guided modes that at those points both $x$ and $y$ components of $(0,0)$th reflected and transmitted order have $\pi$ phase variations. For example $x$ phase variation in Fig. 3(a) at $f_{x_1} = 0.2172$ for $(0,0)$th transmitted order and at $f_{x_2} = 0.2250$ for $(0,0)$th reflected order cannot be considered as guided modes.

If the normalized frequency becomes larger, the phase is no longer constant and starts to vary gradually. This occurs at a boundary point which is the lower boundary of the light cone for these propagation constants. The light cone is a region that includes non-guided or leaky modes and guided modes occur below the light cone and its lower boundary can be calculated separately [11,22]. We also observe that this phenomenon is common in the phase of all diffracted orders. In this example $f_{x_4} = 0.2308$ is the light cone boundary that is evident in Fig. 3(a) and (b).
In structures with mirror symmetry, guided modes can be divided into odd and even modes with respect to the reflections of the horizontal symmetry plane that bisects the structure [10]. We found that when $x$ or $y$ component of the incident wave vector is zero odd or TM-like and even or TE-like, modes are distinguishable by comparing phase of $x$ and $y$ components of reflection and transmission coefficients. When $k_y = 0$ for odd modes phase variations equal to $\pi$ exists only in $x$ components of (0,0)th reflected and transmitted order whereas for even modes this occurs in $y$ components. In the case where $k_y = 0$ the phase variations happen reversely, i.e. odd and even modes are detectable just by $\pi$ phase variations of $y$ and $x$ components of (0,0)th reflected and transmitted order, respectively. For example if the incident propagation constants are considered in the $K \rightarrow \Gamma$ direction as $k_x = 11\pi/15$ and $k_y = 0$. The phase variations of (0,0)th reflected and transmitted order are displayed in Fig. 4. As seen in Fig. 4(a) and (b) $f_N = 0.3322$ demonstrates an odd mode and $f_N = 0.3120$ is an even mode. For these incident propagation constants the lower boundary of the light cone is $f_N = 0.3664$.

4. Results and discussions

In the band structure analysis the incident wave vectors are selected along the different directions of the irreducible Brillouin zone of the hexagonal lattice. One of the possible irreducible Brillouin zone is displaced by a hatched triangle in Fig. 5. The edges of this triangle are $\Gamma \rightarrow M$, $M \rightarrow K$ and $K \rightarrow \Gamma$.
For each pair of Brillouin zone wave vectors \((k_x, k_y)\) reflection and transmission are calculated in various normalized frequencies and the phase variations of \((0,0)\)th diffracted order are monitored. The modes are extracted as explained in the previous section from the phase variations of these coefficients that are equal to \(\pi\). Together, these index-guided modes form the band diagrams. The incident wave vectors \(k_{x1}\) and \(k_{x2}\) which are used in FMM implementation are related to the \(k_x\) and \(k_y\) of the Brillouin zone in this way
\[
\begin{align*}
    k_{x1} &= k_x \\
    k_{x2} &= k_x \sin \delta + k_y \cos \delta.
\end{align*}
\]
where \(\delta = \pi/6\). Also, the \(x\) and \(y\) components of reflected and transmitted coefficients which are necessary in mode extraction are obtained in a similar way using their components in \(x_1\) and \(x_2\) directions that are calculated in Eq. (7).

A free-standing monolayer of polystyrene spheres is considered as first example and its band structures is exhibited in Fig. 6. The contradistinction between odd and even modes in this symmetric structure is possible only for \(K \rightarrow \Gamma\) direction of the Brillouin zone presented in Fig. 5. In other directions \(\pi\) phase variations of modes are the same for both \(x\) and \(y\) components of \((0,0)\)th order. Due to the continuity of bands, the odd or even modes are separable in other directions. If another irreducible Brillouin zone is chosen depending on which edge of the triangle \(k_x\) or \(k_y\) is zero, odd and even modes are recognizable easily as explained in the previous section. The even and odd modes are displayed with squares and circles in Fig. 6, respectively. As illustrated in Fig. 6 there is a band gap for even modes at \(f_q = 0.565 - 0.583\). Also, the lower boundary of the light cone is shown with a dashed line in this band structure.

Note that monolayer colloidal crystals typically needs a substrate to rest on it. Thus, the inverse structure on a substrate with \(\epsilon = 2\) is regarded as second example and its calculated band structure is exhibited in Fig. 7. The inverse structure contains hollow spheres in a medium with refractive index 2.4. This media is \((\text{TiO}_2)\) that recently is used for fabrication of inverse opals [23].

This structure is asymmetric and guided modes cannot be separated into odd and even modes. As seen in its band structure (Fig. 7) the light cone boundary is lower compared to the band structure of a free-standing monolayer polystyrene spheres which is as a result of the presence of substrate. In structures where the refractive index of substrate is greater than the effective refractive index of monolayer colloidal structure, there will be no guided mode below the light cone.

If two-dimensional colloidal crystals or their inverse replicas can be fabricated by other mediums such that the monolayer has higher refractive index contrast, larger band gaps for guided modes can be expected. In these circumstances, the effective refractive index of two-dimensionally periodic colloidal crystal will be higher than the background media. This leads to the confinement of guided modes by total internal reflection in the \(z\) direction and by these two-dimensional gaps light can be confined in the three dimensions [10,11]. This key point can be used in the inexpensive fabrication of devices such as optical waveguides by these structures.

5. Conclusions

Colloidal crystals can be fabricated simply by self-assembly methods in two or three-dimensional periodic arrays, which have attracted much interest as submicron- and nano-scale structures. Two-dimensional colloidal crystals are monolayers of monodisperse colloidal particles that is often self-assembled in hexagonal close packed lattices. We show that index-guided modes of two-dimensional colloidal crystals easily detected by monitoring the phase of \((0,0)\)th reflected and transmitted order. Reflection and transmission coefficients of these three-dimensional nanostuctures are calculated by FMM for different wave vectors of the Brillouin zone. Even and odd modes in structures with mirror symmetry can be specified by comparing the phase of \(x\) and \(y\) components of \((0,0)\)th reflected and transmitted order. The band structures are acquired for a monolayer of polystyrene particles and the inverse replica, i.e. hollow spheres in \((\text{TiO}_2)\) material. This method can be used for fast analysis of 2D colloidal crystals and their inverse replicas with metallic or dielectric substrates.

References


