Symmetry of Two-Dimensional Hybrid Metal-Dielectric Photonic Crystal within Maple

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2D-photonic crystal has the close packed hexagonal structure of metallized spheres. The selection rules are first necessary thing for understanding of interactions between differently polarized light and artificial photonic structure. This problem is the object of our paper. Known methods of group theory allow to solve such problems. However, the knowledge about symmetry of structure is the starting point of them. Usually the X-ray diffraction provides such information about natural 3D-crystals. Such assumptions so far have to do after the visual research of photonic structures in practice. Further these assumptions may be confirmed (or vice versa) by experimental research of optical response of photonic structures. We assumed that the symmetry of photonic structure is close to 2D ($P6mm$) group. Group-theoretical calculations were provided using the system of computer mathematics Maple. Both polarizations, normal to surface and parallel to that plane, were taken into consideration. The obtained selections rules were confirmed later by independent experiments.

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1. Introduction

Hybrid 2D-photonic structure consists of assembling monolayers (MLs) of closely packed colloidal microspheres on a metal-coated glass substrate (Fig. 1). This architecture is one of several realizations of hybrid plasmonic-photonic crystals (PHs), which differ by dimensionality and metal film corrugation [1–3].

We considered this structure as infinite two-periodical layer that lies in a plane (x, y). Axis z is normal to the plane of the layer. Basic translations vectors of the same norm are evidently not normal because have special angle $2\pi/3$. Thus, 2D-elementary cell is correct hexagon (see Fig. 1b) with two spheres inside. It is an approximation obviously, because the real structure is size limited.

The exploring of those properties of structures that are caused by their symmetry was the main goal for us. In particular, it was necessary to establish the so-called "rules of selection". It is the list of allowed transitions between electronic states of different symmetries and energies inducible by light of varying polarization. Additional interest for us was to examine the possibilities of known system of computer mathematics MAPLE 18 within this specific field.

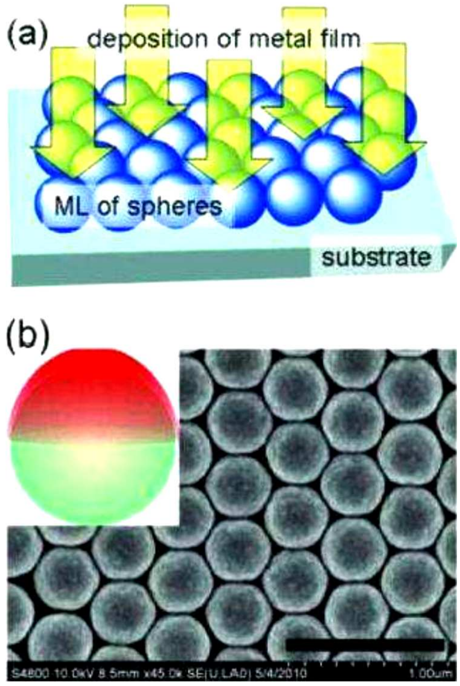

Fig. 1. Artificial two-dimensional plasmonic-photonic crystals [2, 3].

2. Analysis of research and publications

The same norms of both basic translations and specific angle between them define unambiguously a two-dimensional hexagonal primitive lattice. There are only 17 of two-dimensional symmetry groups in general and 13 of them are symmorphic. Just 5 kinds of two-dimensional lattices are known and only one of them is hexagonal primitive [4, 5]. Above-mentioned reasons define unambiguously the group of symmetry of structure shown in Fig. 1.

This group has notation $P6mm$ and belongs to symmorphic groups. It means the presence within this group of a point subgroup (that is $6mm = C_{6v}$), which is isomorphic to factor-group of $P6mm$ group by its translations subgroup.

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Figure 2 shows elements of symmetry of this point subgroup [5]. This group consists of 12 elements of symmetry divided on 6 classes of conjugated elements [4]. Main axis (6) is one-sided, because the symmetry center is absent in $P6mm$ group of symmetry as an independent element. It is normal to the plane of structure.

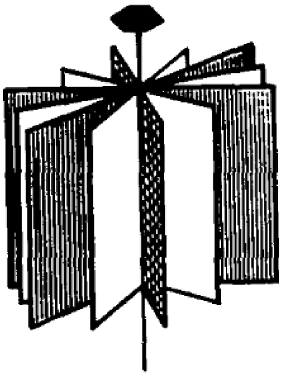

Fig. 2. Elements of $P6mm$ point group of symmetry.

The basic elements of symmetry, or so-called generators, for this point group are two elements: main axis of six-order (C_6) and one of three vertical planes of symmetry (σ_1) of first kind. Figure 2 displays the vertical planes of symmetry of first and second kinds (σ_2) by different way.

3. Methods and results

3.1. Matrix presentation of group elements with Maple

We need only two matrices for generation of all elements of group. They are the matrices of generators of course. Moreover, it should be matrices with (2×2) size because we deal with 2D group. This problem is solvable by LinearAlgebra program package of Maple [1]:

$$C_6 = \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}, \tag{1}$$

$$\sigma_1 = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{2}$$

Now we can easily obtain all another matrices and their traces using command of above package. The clockwise rotation around main axis on angle $5\pi/6$:

$$C_6^5 = (C_6)^{-1}. \tag{3}$$

Two rotations around main axes on angles $\pi/3$ and $2\pi/3$:

$$C_3 = (C_6)^2, \quad C_3^2 = (C_6)^4. \tag{4}$$

One rotation around main axis on the angle $\pi/2$:

$$C_2 = (C_6)^3. \tag{5}$$

Two additional to (2) planes of mirror reflections of first kind

$$\sigma_1^2 = (\sigma_1)^2, \quad \sigma_1^3 = (\sigma_1)^3. \tag{6}$$

Three vertical planes of mirror reflection of second kind

$$\sigma_2 = C_6\sigma_1, \quad \sigma_2^2 = (C_6)^3\sigma_1, \quad \sigma_2^3 = (C_6)^5\sigma_1. \tag{7}$$

Identity element of course

$$E = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{8}$$

All 12 elements of symmetry of group $6mm$ are presented above as matrices.

3.2. Characters of irreducible representations as vectors for $6mm$ group

We could obtain the number of irreducible representations (irreps) and their characters by standard methods of group theory from traces of above matrices. Yet, this has been already done before us [4]. The group has four 1D irreducible representations (A_1, A_2, A_3, A_4) and two 2D (E_1, E_2) according to the well-known Bernside theorem. Therefore, the energy spectra of $P6mm$ structure consist of energy levels of six above-mentioned types of symmetry. Two of them are twice degenerated by symmetry.

We only allowed ourselves to present the characters [4] in a bit unusual, but convenient for calculations of vector forms. According to this A_1 is 1D irreducible representation transform z-components of polar vectors. It may be pulse for instance or normal to plane and longitudinal polarized regarding to the main axis light

$$A_1 = [1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1]. \tag{9}$$

Another 1D-irrep transforms the z-components of an axial vector

$$A_3 = [1, 1, 1, -1, -1, -1, 1, 1, 1, -1, -1, -1]. \tag{10}$$

Such vector may be pulse momentum for example.

Two other 1D-irreps are the following:

$$A_2 = [1, 1, 1, 1, 1, 1, -1, -1, -1, -1, -1, -1], \tag{11}$$

$$A_4 = [1, 1, 1, -1, -1, -1, -1, -1, -1, 1, 1, 1]. \tag{12}$$

First 2D-irrep is

$$E_1 = [2, -1, -1, 0, 0, 0, 2, -1, -1, 0, 0, 0]. \tag{13}$$

The second of them is interesting because transforms the (x, y)-components of polar and axial vectors

$$E_2 = [2, -1, -1, 0, 0, 0, -2, 1, 1, 0, 0, 0]. \tag{14}$$

3.3. Selection rules

3.3.1. Transitions stimulated by longitudinal polarized light

Let the light rays are polarized normal to the plane of structure i.e. longitudinal with respect to main axis of symmetry. Then the perturbation operator transforms according to 1D irreducible representation $A_1 (W = A_1)$.

Let X, Y are characters of irreducible representation according to which it transforms the states belonging to two of six above mentioned energy levels $X, Y \in (A_1, A_2, A_3, A_4)$ and $X[i], Y[i]$ are components of these vectors $(i = 1, 2, ..12)$. Then the transitions $X \leftrightarrow Y$ are allowed at stimulation by operator, which transforms according to the irreducible representation W only under the condition that the sum $\left(\frac{1}{12}\sum_{i=1}^{12} X[i]\cdot W[i]\cdot Y[i]\right)$ is non-zero.

It can be demonstrated that the transitions between states of the same symmetry but different energies are always allowed in this case (Table I).

TABLE I

Allowed transitions for longitudinal polarization.

$A_1 \longrightarrow A_1$:	$\frac{1}{12}\sum_{i=1}^{12} A_1[i]\cdot A_1[i]\cdot A_1[i]=1$
$A_2 \longrightarrow A_2$:	$\frac{1}{12}\sum_{i=1}^{12} A_2[i]\cdot A_1[i]\cdot A_2[i]=1$
$A_3 \longrightarrow A_3$:	$\frac{1}{12}\sum_{i=1}^{12} A_3[i]\cdot A_1[i]\cdot A_3[i]=1$
$A_4 \longrightarrow A_4$:	$\frac{1}{12}\sum_{i=1}^{12} A_4[i]\cdot A_1[i]\cdot A_4[i]=1$
$E_1 \longrightarrow E_1$:	$\frac{1}{12}\sum_{i=1}^{12} E_1[i]\cdot A_1[i]\cdot E_1[i]=1$
$E_2 \longrightarrow E_2$:	$\frac{1}{12}\sum_{i=1}^{12} E_2[i]\cdot A_1[i]\cdot E_2[i]=1$

Any another transitions are obviously prohibited. One of them for example ($E_1 \longrightarrow A_3$) transition is prohibited: $\left(\frac{1}{12}\sum_{i=1}^{12} E_1[i]\cdot A_1[i]\cdot A_3[i]=0\right)$.

Thus the normal to the surface and parallel to the main optical axis polarization of light allowed only transitions between states of the same symmetry but varying energy. The selection rule is extremely simple at the case.

3.3.2. Transitions stimulated by transversal polarized light

The perturbation operator W transforms according to the 2D irreducible representation E_2 at this case ($W = E_2$). Since the selection rules are more complicated (Table II).

TABLE II

Allowed transitions for transversal polarization.

$A_1 \longrightarrow E_2$:	$\frac{1}{12}\sum_{i=1}^{12} A_1[i]\cdot E_2[i]\cdot E_2[i]=1$
$A_2 \longrightarrow E_1$:	$\frac{1}{12}\sum_{i=1}^{12} A_2[i]\cdot E_2[i]\cdot E_1[i]=1$
$A_3 \longrightarrow E_2$:	$\frac{1}{12}\sum_{i=1}^{12} A_3[i]\cdot E_2[i]\cdot E_2[i]=1$
$A_4 \longrightarrow E_1$:	$\frac{1}{12}\sum_{i=1}^{12} A_4[i]\cdot E_2[i]\cdot E_1[i]=1$
$E_1 \longrightarrow A_2$:	$\frac{1}{12}\sum_{i=1}^{12} E_1[i]\cdot E_2[i]\cdot A_2[i]=1$
$E_2 \longrightarrow A_1$:	$\frac{1}{12}\sum_{i=1}^{12} E_2[i]\cdot E_2[i]\cdot A_1[i]=1$
$E_1 \longrightarrow E_2$:	$\frac{1}{12}\sum_{i=1}^{12} E_1[i]\cdot E_2[i]\cdot E_2[i]=1$

The transitions between states with the same symmetry are prohibited at first. There is one of them for instance: $\left(\frac{1}{12}\sum_{i=1}^{12} A_1[i]\cdot E_2[i]\cdot A_1[i]=0\right)$.

4. Conclusions

The software package LinearAlgebra of computer mathematics system MAPLE provides opportunities for calculating energy spectra of hybrid plasmonic-photonic crystals. Thus in such polarization there are allowed some transitions between states of different symmetry and energies in both possible directions. Especially, the transitions are allowed among states with such symmetries

$$\begin{array}{c} A_1 \longleftrightarrow E_2 \longleftrightarrow A_3 \\ \updownarrow \\ A_2 \longleftrightarrow E_1 \longleftrightarrow A_4 \end{array}$$

All conclusions obtained above were confirmed experimentally [2, 3].

Acknowledgments

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References

[1] G.P. Chuiko, O.V. Dvornik, *Symmetry of two-dimensional hybrid metal-dielectric photonic crystal within MAPLE*, Maplesoft, 2013.

[2] S.G. Romanov, N. Vogel, K. Bley, K. Landfester, C.K. Weiss, S. Orlov, *Phys. Rev. B* **86**, 195145 (2012).

[3] S.G. Romanov, A.V. Korovin, A. Regensburger, U. Peschel, *Adv. Mater.* **23**, 2515 (2011).

[4] B.K. Weinstein, in: *Modern Crystallography*, Vol. 1, Eds. B.K. Weinstein, A.A. Chernov, L.E. Shuvalov, Nauka, Moscow 1979, (in Russian).

[5] Y.K. Yegorov-Tismenko, G.P. Litvinskaya, *Theory of Crystal Symmetry*, GEOS, Moscow 2000, (in Russian).