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Molecular Crystals and Liquid Crystals Science and Technology. Section A. Molecular Crystals and Liquid Crystals

Publication details, including instructions for authors and subscription information: http://www.tandfonline.com/loi/gmcl19

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Version of record first published: 24 Sep 2006

To cite this article: G. K. Johri, M. Johria, Tiwari, R. Sharma & Katsumi Yoshino (2001): A Brief Report on Photonic Crystals and Calculations using the Mechanism of Strong Localization of Light, Molecular Crystals and Liquid Crystals Science and Technology. Section A. Molecular Crystals and Liquid Crystals, 368:1, 359-367

To link to this article: http://dx.doi.org/10.1080/10587250108029966

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A Brief Report on Photonic Crystals and Calculations using the Mechanism of Strong Localization of Light

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A brief description of a new class of strongly scattering dielectric microstructures, also called photonic material is given. These crystals are speculated to be of fundamental importance in the present day technology like semiconductors. The main theoretical and experimental developments are given. We have also calculated relative width of the Photonic band gap as a function of refractive index and a comparison is given for the close packed and diamond lattice of fcc 3-D structure. The characteristics of liquid crystal as Photonic crystal are re-analyzed. This work may be fruitful for the investigators in the field of Photonic Crystals.

Keywords: Photonic band gap; Electromagnetic crystal; Photonic crystals; Localization of Light; Spontaneous emission; Dielectric microstructrure

INTRODUCTION

Anderson [1] formulated expressions for the localization of electrons and discussed electron-electron and electron - phonon interactions. The electron localization has already given a breakthrough in the field of Electronics. There existed a question whether there can be any material that perform the same functions with electromagnetic waves (Photons) that semiconductors do with electrons. A number of efforts [2-10] have been made in this direction. A photonic crystal is the optical analogue of an electronic crystal. It is a periodic dielectric structure with its dielectric constant spatially varied according to certain crystal symmetry. Photonic states in photonic crystal depend on bands gaps and, frequency ranges over which optical waves are allowed or forbidden to propagate respectively. The bands and gaps provide a fundamentally new mechanism for steering and localizing light within a semiconductor chip. The understanding of photonic crystals may become easier by their characteristics like lattice structure or lattice constant, shape of the individual atoms.

Our purpose in this paper is two folds, firstly to account briefly for the theoretical and experimental developments in this unexplored field of electromagnetic crystals in three dimensional periodicity and secondly to calculate relative width of Photonic band gap using closed packed and diamond lattice of face centered cubic 3-D dielectric structures.

THEORY

John[2] described that in 3-D two photon mobility edges separate high and low frequency extended states from an intermediate frequency pseudogap of localized states arising from remnant geometric Bragg resonances. Coherent backscattering of light must occur by means of disordered induced within and between such valleys in phase space. The guiding of photon along a particular direction by this remnant of the underline superlattice geometry provides a powerful mechanism for the strong localization of light. Superlattices has been defined as an array of dielectric particles of dielectric constant (ε_a) in a background dielectric constant (ε_b). If we define ε_0 and ε_1 as $\varepsilon_0 = (\varepsilon_a + \varepsilon_b)/2$ and $\varepsilon_1 = (\varepsilon_a + \varepsilon_b)/2$ and $\varepsilon_1 = (\varepsilon_a + \varepsilon_b)/2$

 $(\varepsilon_a - \varepsilon_b)/2$. A significant pseudogap structure in the photon DOS arises when $(\varepsilon_a/\varepsilon_b) \ge 2.13$. Where host is air i.e. $\varepsilon_b = 1$ and the dielectric sphere has dielectric constant $= \varepsilon_a$. The experiments [3] have suggested that materials of high refractive index contrast n_a/n_b favours opening of photonic band gap i.e. (3.5/1) for fcc closed pack structure while theory [5] has predicted 2.1/1 using diamond lattice structure. There are two regions in the dispersion relations predicted by John[2] i.e. a region of $\varepsilon_1/\varepsilon_0 \ge 1/3$ and $\varepsilon_1/\varepsilon_0 \le 1$ which define geometric optic region and Rayleigh scattering and they are separated by pseudo photonic band gap.

John[2] has given realistic picture of the band edge behaviour which require the incorporation of Brillouin zone anisotropy. The wave equation for the classical electric field **E** in a periodic dielectric is given below

$$-\nabla^2 \mathbf{E} + \nabla(\nabla \cdot \mathbf{E}) - (\omega^2/c^2) \, \mathbf{s}_{\text{fluct}}(\mathbf{x}) \, \mathbf{E} = \mathbf{s}_0 \, (\omega^2/c^2) \, \mathbf{E} \tag{1}$$

Where E is electric field amplitude, ω is frequency of monochromatic electromagnetic wave propagating in an inhomogeneous but non dissipative dielectric medium, $\varepsilon(\mathbf{x})$ is total dielectric constant separated into its average value ε_0 and spatially fluctuating part $\varepsilon_{\text{fluct}}(\mathbf{x})$. The value of $\varepsilon_{\text{fluct}}(\mathbf{x})$ plays a role analogous to the random potential $V(\mathbf{x})$ in the Schrödinger equation $\varepsilon_{\text{fluct}}(\mathbf{x})$ scatters the electromagnetic wave. For lossless material, the dielectric constant $\varepsilon(\mathbf{x})$ is real and positive.

John [2] has given solutions of wave equation assuming inversion symmetry as one for high frequency and low frequency and a frequency at the bottom of the frequency as given below

$$\omega/c = \mathbf{k}(\varepsilon_0 \pm \varepsilon_1)^{-1/2} \tag{2}$$

and

$$\omega/c = \mathbf{k}(\varepsilon_0 \pm \varepsilon_1 | 1 - \mathbf{G}^2 / 2\mathbf{k}^2 |)^{-1/2}$$
(3)

Where, ω is frequency; c is speed of light; k is wave vector where $\mathbf{k} = \mathbf{G}/\sqrt{2}$ provided the condition $(\varepsilon_1/\varepsilon_0) \le 1/3$; and G is reciprocal vector. The frequency for the bottom of high frequency is

$$\omega/c = (2\varepsilon_1)^{1/2} \mathbf{G}/(\varepsilon_0 + \varepsilon_1), \quad (\varepsilon_1/\varepsilon_0) > 1/3$$
 (4)

Using these solutions John [2] defined the occurrence of the pseudo photonic gap from the plot of density of states (DOS = $\rho(\omega)$) versus frequency. He has also suggested frequency of the lower branch as

$$\omega/c = \sqrt{(5/12)} \mathbf{G}(\varepsilon_0 + \varepsilon_1/5)^{1/2}$$
 (5)

These solutions have been used for the occurrence of photonic band gap in its intrinsic form.

EXPERIMENT

The experimental effort [3] concentrated on dielectric spheres and on spherical voids in a dielectric background, the spherical – void structure appeared to perform particularly well in this experimental work which is considered to be the first implementation of the idea of photonic band gap. In an another Yablonivitch et al [4] used the same method as described earlier [3].

The crystal structures with Brillouin zones (defined as a Wigner – Seitz cell in the reciprocal lattice) are given in figure 1(a) and (b) for spherical and non-spherical atoms. The Brillouin zone of the non-spherical atoms is identical to the standard fcc BZ.



fcc Brillouin Zone for spherical atom



fcc lattice



fcc Brillouin Zone for non-spherical atom Figure 1. fcc Brillouin Zone and fcc lattice

The photonic band gap material were predicted theoretically as a means to realize two fundamentally optical principles given here in continuation i.e. (1) the localization and trapping of light in bulk material [10], (2) the complete inhibition of spontaneous emission [11] over a broad frequency range. The consequences of these two above principles deal with the photonic band gap.

The fabrication of photonic crystal has been investigated by a number of workers [3,4,12-17] and the problems of infiltrated and tunable photonic crystal have been dealt by Yoshino and his coworkers [18-25]. The idea of Yoshino [22] concerning the experimental realization of the liquid crystal inverse opal structure has been used by Bush and John [26-28]. The tunability of the spontaneous emission, wave guiding effects and light localization enhance the technological utility of liquid crystal photonic band gap materials over and above that of either a bulk liquid crystal or a conventional photonic crystal by itself. It has also been demonstrated [15] that the infiltration of fluorescent and photochromic dyes in to the porous matrix of synthetic opals drastically change the optical properties of the optical dyes.

CALCULATION OF RELATIVE WIDTH AND RE-ANALYSIS OF LIQUID CRYSTAL AS PHOTONIC CRYSTAL

Using expressions (4) and (5) the central frequency (ω_0) can be written as

$$\omega_0 = (\mathbf{Gc/2}) [(2\epsilon_1)^{1/2} (\epsilon_0 + \epsilon_1)^{-1} + (5/12)^{1/2} (\epsilon_0 + \epsilon_1/5)^{-1/2}]$$
 (6)

From the relations (4), (5) and (6) the relative width $(\Delta\omega/\omega_0)$ can be calculated and it is given here below

$$\Delta\omega/\omega_0 = 2\left[\left\{\sqrt{12(n^2-1)(3n^2+2)} - 5n^2\right\} / \left\{\sqrt{12(n^2-1)(3n^2+2)} + 5n^2\right\}\right]$$
 (7)

where we have assumed $\sqrt{\epsilon} \approx n$. The ϵ_0 is $(\epsilon_a + \epsilon_b)/2$, while $\epsilon_1 = (\epsilon_a - \epsilon_b)/2$, where suffix 'a' represents dielectric spheres and 'b' is for the background. We have chosen a case where ϵ_a is varied and $\epsilon_b = 1$. This case suits for dielectric sphere. The relation between wave vector k and reciprocal lattice G is used in the above derivation is

$$\mathbf{k} = \mathbf{G} \left[1 + \left\{ (n^2 + 1) / (n^2 - 1) \right\} \right]^{-1/2}$$
 (8)

Considering n = 3.6 and 2.1 used by Yablonivitch et al [4] and Ho et al [5] for non-spherical atoms fcc closed packed structure and fcc diamond lattice respectively the relative width computed using relation (7) 0.17 for n = 3.6 and 0.12 for n = 2.1.

The plots of variation of $(\Delta\omega/\omega_0)$ versus n are given in Figure 2 for the present calculations using equation (7) and the model of Ho et al [5]. The Table 1 gives the optimal values of refractive index contrast, volume filling fraction, size of the gap in the Photonic crystal in 3-D fcc dielectric crystal structure as determined by different workers [2-5].

The mechanism of density of states minimum used elsewhere [26-28] for the occurrence of Photonic band gap is for isotropic condition which is much more than that for anisotropic behaviour. Johri et al [29] have reported that for anisotropic photonic band gap the size is about 25% to its size for isotropic situation. Bush and John [26,27] assumed the dielectric tensor $\varepsilon(\mathbf{r})$ as given below

$$\varepsilon(\mathbf{r}) = 1 + \varepsilon_{is} \sum_{\mathbf{R} \in \mathbb{R}} S_{is}(\mathbf{r} + \mathbf{R}) + \varepsilon_{LC} \sum_{\mathbf{R} \in \mathbb{R}} S_{LC}(\mathbf{r} + \mathbf{R})$$
(9)

Where S_{is} and S_{LC} describe the location of the optically isotropic backbone and the liquid crystal material within Wigner – Seitz cell. The filling fraction (f) define the following locations.

For
$$f = 9.31\%$$
 to 18.50% $S_{is} = 0$, $S_{LC} = 1$ (10)
For $f = 18.50\%$ to 36.89% $S_{is} = 1$, $S_{LC} = 0$

The relative width varied by varying orientation for nematic liquid crystal BEHA gives maximum relative width [26] as 1.6% by infiltrating silicon with liquid crystal in the ratio about 67 to 100. The refractive index of silicon is considered as 3.45 while principle refractive indices for parallel and perpendicular direction for BEHA are 1.6 and 1.4 respectively with an average of 1.47 which gives negative relative width. Both S_{is} and S_{LC} are zero for f < 9.31% and f > 36.89% while S_{is} and $S_{LC} = 1$ for f = 18.50%. It is the value of

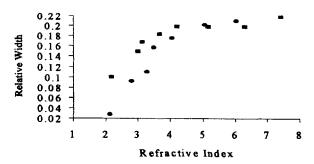


FIGURE 2. Variation of relative width for Present work • using model of Ho et al [5].

TABLE 1. Optimal values of refractive index contrast, volume filling fraction, size of the gap in the photonic crystals in three dimensional fcc crystal structure.

D _a	n/n,	filling fraction (f)	Δαν/σο	Re£	Remark
1.46	1.46			2	Spherical atom and closed packed lattice
1.6	1.6	0.11		3	(pseudogap theoretical) Spherical atom and closed packed
3.5	3.5	0.15	6.7%	3	lattice(experiment-al)
3.06	3.03	0.16	6.7%	3	* *
3.06	3.03	0.67	0.0	3	m m
3.6	3.6	0.37	15.7%	5	Diamond lattice full PBG non- spherical (theoretical)
3.6	3.6	0.81	28.8%	5	
2.0	2.0	0.34(air)	46%	5	# _. #
2.0	2.0	0.81(diele.)	21%	5	* *
3.6	3.6	0.78	19%	4	Cylindrical microstructure closed packed (experimental)
2.1	2.1			4	Normalized hole diameter ≈0.469

filling fraction at which tunability and anisotropy may play important role under the influence of electric field or temperature variation.

CONCLUDING REMARK

It is found that the existence of the photonic band gap in its intrinsic and extrinsic nature have been investigated and band structure as valance band, forbidden band and conduction band have been established theoretically and experimentally but for the full practical impact of PBG structures, which is yet to be seen, require a true mechanism for the occurrence of the PBG and progress in the material science. The present calculation and those using the diamond lattice considered by Ho et al [5] for the occurrence of Photonic band gap give close agreement. The re-analysis and discussion given for liquid crystal to have characteristics of Photonic crystal, their tunability and anisotropic behaviour are of technical importance.

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