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Theoretical study of relative width of photonic band gap for the 3-D dielectric structure

G K JOHRI[1], AKHILESH TIWARI[2], SAUMYA SAXENA[2], RAJESH SHARMA[2], KULDEEP SRIVASTAVA[2] and MANOJ JOHRI[1]
[1]Department of Physics and Electronics, D.A.V. College, 119/91, Darshanpurwa, Kanpur 208 012, India
[2]Dr. Virendra Swarup Centre of Applied Science and Technology, Kanpur 208 001, India
Email: dvs_cast12@yahoo.com; tiwaria_1999@yahoo.com

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Abstract. Calculations for the relative width $(\Delta\omega/\omega_0)$ as a function of refractive index and relative radius of the photonic band gap for the fcc closed packed 3-D dielectric microstructure are reported and comparison of experimental observations and theoretical predictions are given. This work is useful for the understanding of photonic crystals and occurrence of the photonic band gap.

Keywords. Photonic band gap; photonic crystal; dielectric microstructure.

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1. Introduction

The challenge of controlling and manipulating light by opening a gap in the photon density of states with a given range of frequencies could be met by an artificially fabricated photonic crystal within which a defect in the periodicity is required rather than a naturally available perfect crystal. It is known from the literature [1–3] that three-dimensional (3-D) periodic dielectric structures called photonic crystals (PCs) exhibit frequency forbidden gap and the experimental verification have been reported earlier [3]. Ho *et al* [2] have given 3-D complete photonic band gap (CPBG), where Yablonovitch *et al* [3] have fabricated PCs for the microwave region. The investigators [4–6] have also reported designs for CPBG. The possibility of artificial fabrication of dielectric structure for light emission inside the PC has potential technical applications. Although Jaonnopoulos [5] and other workers [6] have given a summary of the work in this field and it is emerging as non-conventional systems, there is a need to look into the basics of this field as their qualitative comparison may pave the way to facilitate understanding about occurrence of the photonic band gap (PBG). We are motivated to compute the variations of relative width $(\Delta\omega/\omega_0)$ as a function of refractive index contrast $(n_a/n_b$ with $n_a = n$ and $n_b = 1)$, using John [1]

model and computed values are qualitatively compared with those predicted theoretically [1,2] and observed experimentally [3].

2. Theoretical details

A realistic picture of band edge behaviour requires the incorporation of Brillouin-zone (BZ) anisotropy. John [1] used the wave equation for the classical electric field **E** in a periodic dielectric given as

$$-\nabla^2\mathbf{E} + \nabla(\nabla\cdot\mathbf{E}) - (\omega^2/c^2)\varepsilon_{\text{fluct}}(\mathbf{x})\mathbf{E} = \varepsilon_0(\omega^2/c^2)\mathbf{E}, \tag{1}$$

where **E** is the electric field, ω the frequency of monochromatic electromagnetic wave propagating in an inhomogeneous but non-dissipative dielectric medium and $\varepsilon(\mathbf{x})$ the total dielectric constant separated into average values 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. The $\varepsilon_{\text{fluct}}(\mathbf{x})$ scatters EM wave. For lossless material the dielectric constant $\varepsilon(\mathbf{x})$ is real and positive. Unlike the familiar picture of electronic localization, what we are really seeking when searching for localized light is an intermediate frequency window within the positive energy continuum that lies at energy higher than the highest of the potential barriers. It is for this simple reason that ordinary dielectrics appearing in nature do not easily localize light. The $\varepsilon_0(\omega^2/c^2)$ is an eigenvalue when compared with Schrödinger equation and its value is always greater than $|(\omega^2/c^2)\varepsilon_{\text{fluct}}(\mathbf{x})|$ for the condition $(\varepsilon_0 + \varepsilon_{\text{fluct}}) > 0$.

In eq. (1) the fluctuating part of the dielectric constant describes a fcc lattice of spheres

$$\varepsilon_{\text{fluct}}(\mathbf{x}) = \varepsilon_1 \sum_{\mathbf{G}} U_{\mathbf{G}} \exp(j\mathbf{G}\cdot\mathbf{x}), \tag{2}$$

where **G**'s are the reciprocal lattice vectors. The nearly free photon approximation follows from treating $\varepsilon_{\text{fluct}}$ as a small perturbation relative to ε_0. $\varepsilon_0 = (\varepsilon_a + \varepsilon_b)/2$ and $\varepsilon_1 = (\varepsilon_a - \varepsilon_b)/2$ where ε_a is for dielectric sphere and ε_b is for the background. There may be two cases: (i) $\varepsilon_a =$ varied, $\varepsilon_b = 1$ for dielectric sphere and (ii) $\varepsilon_a = 1$, $\varepsilon_b =$ varied for air atoms. The dielectric contrast is defined by $(\varepsilon_a/\varepsilon_b)$ and refractive index contrast by (n_a/n_b) with $\sqrt{\varepsilon} = n$.

Setting the dominant Fourier component $U_G = 1$, the Bragg scattering of photons from wave vector **k** to $\mathbf{k} - \mathbf{G}$ leads to the following approximate but realistic solutions of eq. (1) using 4th order determinant. These solutions are given below:

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

and

$$\omega = c\mathbf{k}(\varepsilon_0 \pm \varepsilon_1|1 - G^2/2\mathbf{k}^2|)^{-1/2}. \tag{4}$$

Equation (1) corresponds to the polarization vector lying out of the plane (s-polarization) and in the plane (p-polarization) of Bragg scattering. For $(\varepsilon_1/\varepsilon_0) > 1/3$, the phase space (allowed values of **k**) for propagation near a band edge is determined by the p-polarization

channel. In these equations c is the speed of light and $\mathbf{k}$ is the wave vector where $k = G/\sqrt{2}$ for $(\varepsilon_1/\varepsilon_0) \leq 1/3$. The angular frequencies for the width calculations are

$$\omega = (2\varepsilon_1)^{1/2} G/(\varepsilon_0 + \varepsilon_1), \quad \text{for } (\varepsilon_1/\varepsilon_0) \geq 1/3, \tag{5}$$

$$\omega = (5/12)^{1/2} G/(\varepsilon_0 + \varepsilon_1/5)^{1/2}, \tag{6}$$

where $(\mathbf{k}^2/\mathbf{G}^2) = 5/12$.

We have computed relative width $(\Delta\omega/\omega_0)$ with ω_0 as central frequency in terms of refractive indices assuming $n_b = 1$ and $n_a =$ varied for closed packed lattice of the fcc structure for dielectric spheres. The central frequencies ω_0 were obtained by taking the mean values of frequencies of upper edge and lower edge of the pseudo photonic band gap within the framework of John's formulation [1]. The center angular frequency (ω_0) from eq. (6) is given by

$$\omega_0 = (\mathbf{G}/4)(5/3)^{1/2}[(\varepsilon_0 - \varepsilon_1/5)^{-1/2} + (\varepsilon_0 + \varepsilon_1/5)^{-1/2}]. \tag{7}$$

The values of $\Delta\omega/\omega_0$ are

$$\Delta\omega/\omega_0 = 2\left[\left\{\sqrt{(3n_a^2 + 2n_b^2)} - \sqrt{(2n_a^2 + 3n_b^2)}\right\} \Big/ \left\{\sqrt{(3n_a^2 + 2n_b^2)} + \sqrt{(2n_a^2 + 3n_b^2)}\right\}\right]. \tag{8}$$

3. Results and discussion

The computed values of relative width as a function of refractive index contrast n_a/l for eq. (8) is shown in figure 1. The variations of $(\Delta\omega/\omega_0)$ computed by Ho *et al* [2] for dielectric spheres and air atoms are given for comparison in figure 2.

An examination of figure 1 shows that $(\Delta\omega/\omega_0)$ given by eq. (8) varies almost similar to dielectric spheres as those proposed by Ho *et al* [2] and given in figure 2. These two models are based on fcc closed packed structure [1] and diamond lattice [2] using spherical structure. Equation (8) gives a saturated value of $(\Delta\omega/\omega_0) \approx 13\%$ at about $n_a = 2.0$, which is the threshold value reported by Ho *et al* [2]. The saturated values of $(\Delta\omega/\omega_0)$ are 21% and 46% [2] for dielectric spheres and for air atoms respectively, using the diamond lattice as illustrated in figure 2. It is found that eq. (8) for $(\Delta\omega/\omega_0)$ versus n_a is in close agreement with that for dielectric sphere while experimental values [3] range in the region where Ho *et al* [2] predicted for air atoms. We find the limits of refractive index in the range 2.1/1 to 3.6/1 for the opening of the photonic band gap and for the end of it. Equation (8) give $\Delta\omega/\omega_0 = 13\%$ for 2.1 and $\Delta\omega/\omega_0 = 17\%$ for 3.6. For a common refractive index of 3.6 and W point of the BZ as considered by Yablonovitch *et al* [3] and also by Ho *et al* [2] $\Delta\omega/\omega_0$ is 17% and 15% considering non-spherical atoms and diamond lattice respectively as given in figure 1.

The ratio first increases between refractive index 2 to 2.8 and after $n = 3.0$ there is saturation and the ratio of calculated relative width by John's model [1] and the model of Ho *et al* [2] become almost independent of refractive index contrast. The difference between these

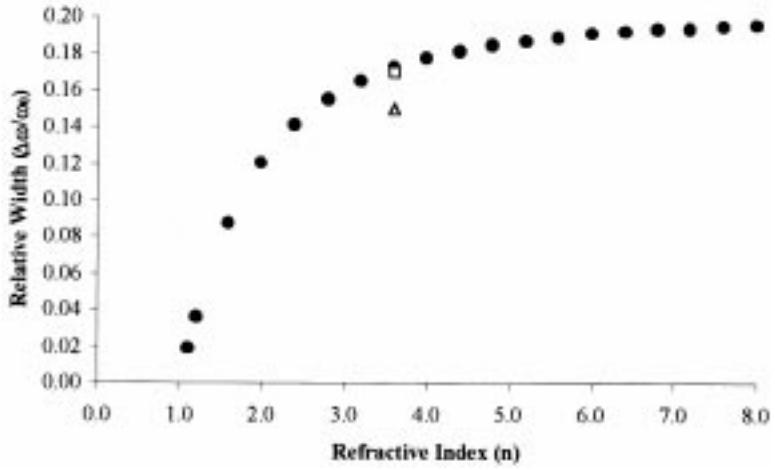

Figure 1. Variation of relative width $(\Delta\omega/\omega_0)$ with refractive index (n) for eq. (8); □ – Yablonovitch [3]; Δ– for Ho *et al* [4].

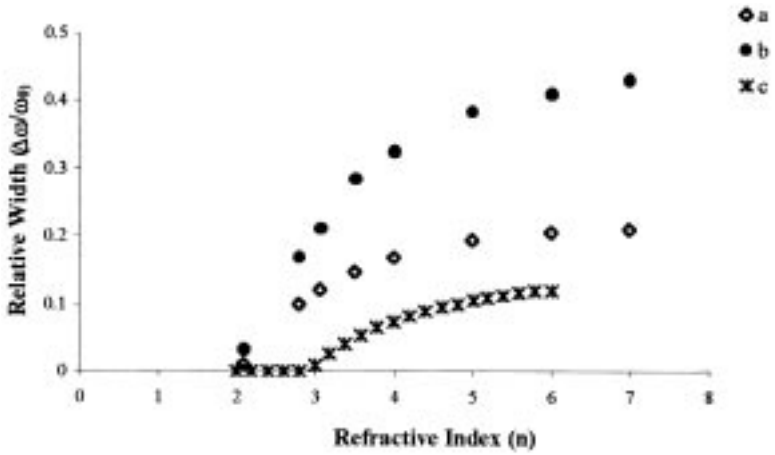

Figure 2. Variation of relative width $(\Delta\omega/\omega_0)$ with refractive index (n) for (a) dielectric sphere, (b) air atom both due to Ho *et al* [2] and for (c) inverted fcc structure.

two models appears to be around 18%, which may be merely due to assumptions of closed packed lattice and diamond lattice but in both these cases spherical atoms are considered. In addition to the variation of relative width with refractive index an additional parameter of filling fraction or relative radius is also important to see its effect on the relative width [2] but it has not been considered in our present calculations.

4. Conclusions

From the work reported it is found that although the work of Ho *et al* gives lower limit to the refractive index contrasts $(n/1 \approx 2)$ for complete photonic band gap using diamond lattice in comparison to the experiment $(n/1 \approx 3.5)$, it is too hard to fabricate a PC, while the concept of John for fcc closed packed structure used in this work for pseudogap photonic band gap is fruitful and realistic to understand the occurrence of PBG. This calculation gives emergence of pseudogap at refractive index contrast $(n/1 \approx 1/2)$. The present comparison although qualitative is useful to know the variation of relative width in terms of the important parameters like refractive index contrast.

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