Study on the Photonic Band Gaps of the Face Centered Cubic Crystals

K.B.S.K.B. Jayawardana^{1,a}, K.A.I.L. Wijewardena Gamalath^{2,b*}

^{1,2}Department of Physics, University of Colombo, Colombo 03, Sri Lanka.

^asunethjayawardana@gmail.com, ^bimalie@phys.cmb.ac.lk

Keywords: Photonic crystal, face centered cubic, plane wave expansion method, band gap, dielectric contrast, filling factor, gap to mid gap ratio, mode field distribution

Abstract. Since the dielectric contrast of photonic crystals play an important role in determining the existence of a photonic gap, the photonic energy bands, density of states of face centered cubic structured photonic crystals formed from spheres of several dielectric materials placed in air were calculated using the plane wave expansion method. A complete band gap was obtained between second and third bands with a gap to mid gap frequency ratio in the range 3.59–5.37% for the dielectric contrast in the range 11–16 with dielectric spheres of radius $r = 0.2a$ with a filling factor of 0.134 and for dielectric contrast of 200 with $r = 0.3a$. A complete gap was not found for the dielectric contrast of 3.9. A complete band gap can be obtained for filling factors 0.057–0.26 for the dielectric contrast in the range 11–16 with an optimum band gap for the filling factor 0.134 while GaAs ($\epsilon = 13.1$) has almost a constant optimum band gap in this range. The largest gap to mid gap ratio of 5.37% was obtained for GaP ($\epsilon = 11.1$). For dielectric spheres of $r = 0.15a$, $0.20a$ and $0.25a$ larger gap to mid gap ratio were obtained for the dielectric contrast 11–12.5 while the largest were obtained for $r = 0.2a$. The only dielectric material BaSrTiO₃ ($\epsilon = 200$) which gives a band gap for the filling factor of 0.4524 can be used in microwave applications.

1. Introduction

The optical analogue of an ordinary crystal is a three dimensional photonic crystal, an artificially formed dielectric structure periodic along the three axes. When electromagnetic waves interact with these crystals as they periodically modulate the dielectric constant, a photonic band gap may form in these directions prohibiting the propagation of photons for energies that lie within the gap. Under certain conditions, there will be regions of forbidden frequencies for all the directions of propagation, creating a full photonic band gap. Only the three dimensional photonic crystals may possess a complete photonic band gap in all directions, which is significant for optical or optoelectronic device operations in radio to optical wavelengths [1]. In this energy band, optical modes, spontaneous emission, and zero point fluctuations are all absent. The scattering strength in the crystal may be assessed qualitatively by the refractive index contrast between the two materials, specifically by the ratio of their refractive indices. The photonic band theory is essentially exact since photon interactions are negligible [2].

One century after Lord Rayleigh [3] in 1887 described the one dimensional photonic band gaps, the possibility of a three dimensional photonic band gaps in periodic structures was suggested by Yablonovitch [4]. Three years later Ho et al. [5] correctly predicted a specific dielectric structure having a complete band gap. Based on theoretical calculations many structures have been fabricated and characterized with band gaps at wavelengths ranging from microwave to infrared regimes. The most natural real-space structure for the optical medium is face centered cubic (fcc), which is the most well-known atomic arrangement in crystals. Earlier research [2,6] had indicated that it is desirable for the Brillouin zone in reciprocal space to be as near to spherical as possible and the lowest-order Brillouin zone for the fcc structure is closer to spherical than the Brillouin zones of any other common crystal structures [2]. Periodic dielectric structures possessing large photonic band gaps have been based primarily on face-centered-cubic and diamond symmetry [7]. The first experimental results published for fcc lattice of polycrystalline Al₂O₃ spheres 6 mm in diameter, with a microwave refractive index of 3.06, in thermal-compression-moulded dielectric foam of

refractive index 1.01 indicated the presence of a ‘photonic band gap’ in the microwave regime [8]. Although subsequent numerical calculations [9,10] using the plane-wave method supported the claim that no gap opens in the spectrum and only a pseudo-gap exists, two years later Sozuer et.al [11] found a full gap for the fcc lattice of dielectric spheres between the eighth and ninth bands. Later, these results were confirmed by two other groups [12,13] using the plane-wave method. The photonic analogue of the Korringa-Kohn-Rostoker method is a viable alternative to the plane-wave method for analysing the spectrum of electromagnetic waves in a three-dimensional fcc lattice formed from homogeneous dielectric spheres [14].

The dielectric contrast of the two mediums play important role in determining the photonic gap. Therefore, the plane wave expansion method developed for bcc [15] lattice applicable to any type of non-dispersive dielectric functions was used as the numerical technique in modeling and simulating the band structures of three dimensional fcc structured photonic crystals formed by dielectrics spheres of Si and Ge of group IV; GaP, InAs, GaAs, InP of group III-V; SiO₂ and BaSrTiO₃ spheres placed in air. Barium-strontium titanate (BaSrTiO₃) was selected as it is a favorable electronic material because of its high dielectric constant and variable Curie temperature with composition [16]. For the periodic dielectric function, the magnetic field vector was expanded using Bloch theorem leading to eigenvalue equation in matrix form. Standard eigenvalue equation was solved for the lattice geometries and the energy band and density of states were calculated for the eight materials using Matlab for 343 plane waves with lattice constant taken as one unit. For the fcc structures constructed with air spheres as localized medium with the dielectrics as the background medium, there were only partial band gaps. The materials with smaller dielectric constants did not give any kind of a band gaps, but distorted the symmetry of the band diagram. The photonic band structure for a close-packed fcc lattice formed from dielectric spheres in air, a band gap was obtained between second and third bands with a mid-gap frequency ratio of about 5% for GaP, Si, InP and InAs and about 4% for GaAs and Ge. For BaSrTiO₃ spheres placed in air, a photonic gap with gap to mid gap frequency ratio of about 5% was obtained only for filling factor of 0.452. For the propagation of telecommunication waves in the fcc photonic crystal formed by GaP spheres in air, the mode field distributions for TM and TE modes at the symmetric points X, U, L, Γ, X, W, K of the irreducible Brillouin zone are presented using finite difference time domain method using OptiFDTD software package [17] developed by Opticwave.

2. Materials and Method

The propagation of light in a photonic crystal is governed by the four Maxwell equations. The photonic crystal was considered to be a macroscopic, homogeneous, isotropic dielectric material with real dielectric constant $\epsilon(\mathbf{r})$ without dispersion, placed charges or current densities. For anisotropic dielectric material, the magnetic permeability is $\mu(\mathbf{r}) \approx 1$. By combining the source-free Faraday’s and Ampere’s laws at a fixed angular frequency ω with harmonic time dependence of the electric field and magnetic field strength leads to the master equation for a periodic dielectric structure. There are several methods for solving a photonic band structure and the most customary and popular methods are the plane wave expansion method (PWE) and finite difference time domain method (FDTD). In plane wave expansion method, a set of plane waves are used to expand, the periodic functions in a Fourier series. Because of the periodic nature of photonic crystals, the magnetic field is expanded into a sum of plane waves in reciprocal space giving an arbitrary spatial frequency call reciprocal lattice vector $\mathbf{G}_i = h_i \mathbf{b}_i$ in terms of basis vectors $\mathbf{b}_i$ in the reciprocal space and set of are integers h_i leads to the equation [15]:

$$\sum_{\mathbf{G}'} |\vec{k} + \vec{G}| |\vec{k} + \vec{G}'| \epsilon^{-1}(\vec{G} - \vec{G}') \begin{bmatrix} \hat{e}_2 \cdot \hat{e}_2' & -\hat{e}_2 \cdot \hat{e}_1' \\ -\hat{e}_1 \cdot \hat{e}_2' & \hat{e}_1 \cdot \hat{e}_1' \end{bmatrix} \begin{bmatrix} h_1' \\ h_2' \end{bmatrix} = \begin{bmatrix} M_1 & M_2 \\ M_3 & M_4 \end{bmatrix} \begin{bmatrix} h_1(G') \\ h_2(G') \end{bmatrix} = \frac{\omega^2}{c^2} \begin{bmatrix} h_1 \\ h_2 \end{bmatrix} \quad (1)$$

where $\hat{e}_\lambda$ are two orthogonal unit vectors perpendicular to $\mathbf{k} + \mathbf{G}_i$. The dielectric function of the structure is similarly expanded in terms of reciprocal lattice vectors: Fourier transformation of the dielectric function $\varepsilon(\mathbf{G})$ is given by

$$\varepsilon(\mathbf{G}) = \begin{cases} f\varepsilon_a + (1-f)\varepsilon_b & \text{for } \mathbf{G} = 0 \\ (\varepsilon_a - \varepsilon_b)S(\mathbf{G}) & \text{for } \mathbf{G} \neq 0 \end{cases} \quad (2)$$

where ε_a and ε_b refer to the dielectric constants of the localized medium and background respectively. f is the filling factor defined as the fraction of area occupied by the localized medium in one unit cell. The factor $S(\mathbf{G})$ relying on the geometry of the localized medium and the lattice structures for a three dimensional sphere with radius R is given by:

$$S(G) = 3f \left[\frac{\sin(GR) - GR \cos(GR)}{(GR)^3} \right] \quad (3)$$

The transverse $\mathbf{D}$ field is given by [15]:

$$\mathbf{D}_k^w(\mathbf{r}) = \frac{1}{|\mathbf{k}|} \sum_{\mathbf{G}} |\mathbf{k} + \mathbf{G}| h_1(\mathbf{G}) \cdot e^{i(\mathbf{k} + \mathbf{G}) \cdot \mathbf{r}} \hat{\mathbf{z}} \quad (4)$$

and the transverse $\mathbf{H}$ field is given by:

$$\mathbf{H}_k^w(\mathbf{r}) = \sum_{\mathbf{G}} h_1(\mathbf{G}) \hat{\mathbf{z}} \cdot e^{i(\mathbf{k} + \mathbf{G}) \cdot \mathbf{r}} \quad (5)$$

The face centered cubic (FCC) crystal structure with a lattice constant a and the irreducible Brillouin zone is shown in figure 1(a) and 1(b) respectively. The Lattice vectors are given by $\mathbf{a}_1 = a(0, 1, 1)/2$, $\mathbf{a}_2 = a(1, 0, 1)/2$, and $\mathbf{a}_3 = a(1, 1, 0)/2$. The symmetric points in the irreducible Brillouin zone are $\Gamma = (0, 0, 0)$, $X = (0, 1, 1)/2$, $K = (3, 6, 3)/8$, $U = (2, 5, 5)/8$, $W = (1, 3, 2)/4$, and $L = (1, 1, 1)/2$. The fcc structured photonic crystal was formed by replacing the atoms in the primitive cell with dielectric spheres in air as shown in figure 1(c) so that the dielectric constants for localized medium ($\varepsilon_a = \varepsilon$) and background material ($\varepsilon_b = 1$) or by drilling air spheres ($\varepsilon_a = 1$) in dielectric mediums ($\varepsilon_b = \varepsilon$).

Fig. 1: (a) FCC Lattice, (b) irreducible Brillouin zone and (c) FCC Lattice formed by replacing atoms with dielectric spheres

The number of grid points n in the direction of each basis lattice vector in space were specified in a three dimensional grid. The number of grid points or plane waves used was $(2n+1)^3$. Defining the number of plane waves as 343, the reciprocal grid was formed. After specifying the high symmetrical points in the three dimensional geometry, all the coefficients in the matrix M given in equation 1 were formed by calculating two unit vectors. Lattice constant was taken as one

($a = 1$ 'unit'). The radius of the dielectric sphere R was changed until the closed packed filling factor of 0.74 ($R = a/2\sqrt{2} = 0.35a$) was obtained. All the eigenvalues for the matrix were calculated for each $\mathbf{k}$ vector in the first irreducible Brillouin zone.

3. Results

For fcc structured photonic crystals formed from spherical air holes in all the dielectric materials, a complete band gap was not found, although there were partial band gaps. Hence these are not presented. In the case of fcc structured photonic crystals formed from dielectric spheres in air, the radii of the dielectric spheres for each material were changed until optimum band gap was obtained. SiO_2 ($\epsilon = 3.9$) dielectric spheres in air did not give any complete or partial band gaps for the filling factor in the range of 0.016–0.740 with variation of the radius of the spheres $(0.10 - 0.35)a$.

The calculated energy bands and density of states for optimum band gaps obtained in symmetric directions X, U, L, Γ, X, W, K of the irreducible Brillouin zone of the face centered cubic, formed from dielectrics spheres of radius $R = 0.20a$ from GaP, Si, InP, GaAs, InAs and Ge drilled in air having a filling factor of 0.134 are shown in figures 2-7 for normalized frequency $\omega a / 2\pi c = a / \lambda$. The yellow region indicates a complete gap. Figure 2 shows the energy bands and density of states of GaP ($\epsilon = 11.1$) photonic crystal. This has a complete band gap of $0.0292 \omega a / 2\pi c$ between second and third bands and the gap to mid gap frequency ratio ($\Delta\omega / \omega_{mid}$) is 5.37%. There are partial band gaps between every two adjacent bands from third to seventh bands. This largest complete band gap given by GaP crystal among different filling factors is very small. The lattice dimensions vary according to the size of the wavelength that propagate through the lattice.

Fig. 2: Band diagram (left) and normalized DOS (right) of GaP ($\epsilon = 11.1$) for $R = 0.20a$

Energy bands and density of states of fcc photonic crystals formed from Si ($\epsilon = 11.68$) spheres of radius $R = 0.20a$ in air is presented in figure 3. This fcc Si lattice has the filling factor of 0.134 as GaP. The optimum band gap of $0.0280 \omega a / 2\pi c$ was obtained between second and third band and there are partial band gaps between third to seventh adjacent bands. The gap to mid-gap ratio ($\Delta\omega / \omega_{mid}$) is 5.27% for the complete band gap. Figures 4, 5, 6 and 7 show the energy bands and density of states of fcc crystal formed from InP ($\epsilon = 12.4$), GaAs ($\epsilon = 13.1$), InAs ($\epsilon = 14.6$) and Ge ($\epsilon = 16.0$) spheres of radius $R = 0.20a$ in air for optimum complete band gaps respectively. For the filling factor of 0.134, these lattices have complete band gaps of 0.0268, 0.0181, 0.0234 and

0.0188 in normalized frequency between second and third bands and the gap to mid gap frequency ratios are 5.21%, 3.59%, 4.93% and 4.14% respectively. There are partial band gaps for InP and Ge between third to sixth adjacent bands. For GaAs and InAs partial band gaps are present only between third and fourth bands.

Fig. 3: Band diagram (left) and normalized DOS (right) of Si ($\epsilon = 11.68$) for $R = 0.20a$

Fig. 4: Band diagram (left) and normalized DOS (right) of InP ($\epsilon = 12.4$) for $R = 0.20a$

Fig. 5: Band diagram (left) and normalized DOS (right) of GaAs ($\epsilon = 13.1$) for $R = 0.20a$

Fig. 6: Band diagram (left) and normalized DOS (right) of InAs ($\epsilon = 14.6$) for $R = 0.20a$

Fig. 7: Band diagram (left) and normalized DOS (right) of Ge ($\epsilon = 16$) for $R = 0.20a$

BaSrTiO₃ ($\epsilon = 200$) only give a complete band gap of $0.0042 \omega a / 2\pi c$ between second and third band for filling factor of 0.452 with dielectric spheres of radius $0.3a$ drilled in air. This is the only band gap given by BaSrTiO₃ and is shown in figure 8 by the yellow region. The gap to mid-gap ratio ($\Delta\omega / \omega_{mid}$) is 4.71%. There are partial band gaps between third to sixth adjacent bands.

Fig. 8: Band diagram (left) and normalized DOS (right) of BaSrTiO₃ ($\epsilon = 200$) for $R = 0.30a$

From these energy band diagrams, the gap widths and the mid gap widths were obtained for each fcc material. For the telecommunication wave length $\lambda = 1.55\mu\text{m}$, the lattice constants were obtained from the mid gap position a/λ . The radius of sphere for each type of fcc material and filling factor and lattice constant with the width to mid gap ratio for these photonic crystals for telecommunication wavelength are presented in table 1. For telecommunication industry gallium phosphide (GaP) is the most promising fcc photonic crystal among others due to its highest band gap and highest gap to mid gap ratio. BaSrTiO₃ is the only material which gives a band gap when the filling factor is 0.4524 and thereby using this material though it is possible to create a larger photonic crystal compared to the other dielectric materials the band gap is too narrow ($4.16 \times 10^{-3} \omega a / 2\pi c$). For telecommunication wavelength of $1.55\mu\text{m}$, BaSrTiO₃ gives a lattice constant of 136.4nm and the radius of a dielectric sphere is 41nm . As these values are in nanometer scale it is hard to design a photonic crystal. If BaSrTiO₃ photonic crystal is used in microwave region then the lattice constant will vary from $4.16\mu\text{m}$ to 4.16mm range and can be used in microwave applications.

Table 1: Lattice parameters, dielectric constants and band gaps for telecommunication wavelength

Material	Dielectric constant	Lattice constant [μm]	Radius of the sphere [μm]	Filling factor	Band gap [$\omega a / 2\pi c$]	Gap/ mid gap frequency ratio
GaP	11.1	0.8421	0.168	0.134	0.0292	5.37%
Si	11.68	0.8210	0.164	0.134	0.0280	5.27%
GaAs	13.1	0.7810	0.156	0.134	0.0181	3.59%
InAs	14.6	0.7350	0.147	0.134	0.0234	4.93%
InP	12.4	0.7970	0.159	0.134	0.0268	5.21%
Ge	16.0	0.7046	0.140	0.134	0.0188	4.14%
BaSrTiO ₃	200	0.1364	0.041	0.452	0.0042	4.71%

4. Gapwidth with dielectric function and filling factor

The existence and size of a photonic band gap depend on the symmetry of the photonic crystal as well as on the contrast in the magnitude of the refractive indices between the constituent materials in the system. The gap width depends on the filling factor and therefore the variation of gap width with the filling factor for the materials which gave complete band gaps were calculated and these are presented in figure 9. GaP, Si, InP, GaAs, InAs and Ge gives the maximum band gaps for filling factor in the region 0.057 to 0.26. Except for the GaAs, the complete band gaps of all the other dielectric materials with the filling factor resemble a F distribution. GaAs has nearly a constant band gap of $0.0181 \omega a / 2\pi c$ in the range of spherical radius $r = (0.15 - 0.25)a$ and filling factor 0.0565 – 0.2618.

The variation of the gap to mid-gap ratio ($\Delta\omega / \omega_{mid}$) of the complete band gap obtained for fcc structured photonic crystal with the dielectric contrast and filling factors calculated for spheres of radiuses $0.15a$, $0.20a$ and $0.25a$ are shown in figure 10. When the dielectric spheres are of radius $r = 0.15a$ the optimum band gap is obtained for $\varepsilon = 13 - 15$, $r = 0.2a$ for $\varepsilon = 11 - 12.5$ and $r = 0.25a$ for $\varepsilon = 12.5 - 13$ with $r = 0.2a$ giving the highest band gaps. When filling factor is about 0.134 the largest gap-to-mid-gap ratio of 5.37 % is obtained for GaP with dielectric contrast of 11.1. For the filling factor of 0.262, the maximum mid gap ratio is for InP with dielectric contrast of 12.4. When the filling factor is 0.0565 the two materials GaAs and InAs give approximately same size of gap to mid gap ratio of 2.82% for dielectric contrast of 13.1 and 14.6 respectively.

Fig. 9: Variation of gap width with filling factor for GaP, Si, InP, GaAs, InAs and Ge FCC photonic crystals

Fig. 10: Variation of gap width to mid gap ratio with dielectric constant for dielectric spheres of radii $0.15a$, $0.20a$ and $0.25a$

In order to obtain the optimum band gap, the filling factors of the fcc structured photonic crystals formed from GaAs, GaP, InP and BaSrTiO₃ spheres in air for the wavelength range 1550 nm – 1 mm is given in table 2. These fcc structured photonic crystal can also be used in radio wave frequency for the wavelength range of 1 mm – 100,000 km. The range of the lattice constants for different radio wavelength bands such as extremely high frequency, EHF (1 mm – 1 cm), super high frequency, SHF (1 cm – 10 cm), ultra-high frequency, UHF (10 cm – 1 m) and very high frequency, VHF (1 m – 10 m) are tabulated in table 3.

Table 2: Optimum band gap materials and filling factors for fcc structure for wavelength range 1550 nm – 1 mm

Optimum gap [$\omega a/2\pi c$]	Filling factor	Range of the lattice constant	Dielectric material
0.0186	0.057	1.02 μm – 0.66 mm	GaAs
0.0292	0.134	0.84 μm – 0.54 mm	GaP
0.0194	0.262	0.64 μm – 0.41 mm	InP
4.16×10^{-3}	0.452	0.14 μm – 0.09 mm	BaSrTiO ₃

Table 3: Optimum band gap materials and filling factors for fcc structure for EHF, SHF, UHF and VHF ranges

Dielectric material	GaAs	GaP	InP	BaSrTiO ₃
Optimum gap in [$\omega a/2\pi c$]	0.0186	0.0292	0.0194	4.16×10^{-3}
Filling factor	0.057	0.134	0.226	0.452
Lattice constant for EHF [1mm – 1cm]	0.66mm–0.66cm	0.54mm–0.54cm	0.41mm–0.41cm	0.09mm–0.09cm
Lattice constant for SHF [1cm – 10cm]	0.66cm – 6.6cm	0.54cm – 5.4cm	0.41cm – 4.1cm	0.09cm – 0.9cm
Lattice constant for UHF [10cm – 1m]	6.6cm – 0.66m	5.4cm – 0.54m	4.1cm – 0.41m	0.9cm – 0.09m
Lattice constant for VHF [1m – 10m]	0.66m – 6.6m	0.54m – 5.4m	0.41m – 4.1m	0.09m – 0.90m

5. Wave propagation through gap fcc photonic crystal

Fig. 11: (a) Distribution of atoms in GaP FCC lattice with a filling factor of 0.134, (b) Spreading of dielectric constant over x-z plane

Fig. 12: The 3D view of the propagation variation of amplitudes of (a) E_z and (b) H_z for TM and TE modes at Γ and K points in GaP FCC photonic lattice with a filling factor of 0.134

The spreading of the dielectric constant over x-z plane for a fcc crystal formed from GaP spheres of radius $R=0.2a$ in air with a filling factor of 0.134 is shown in figure 11. When an electromagnetic wave with wavelength $1.55\mu\text{m}$ that is a telecommunication wave was propagated through this photonic crystal lattice, the electric field components E_x, E_y, E_z and magnetic field components H_x, H_y, H_z were obtained. The three dimensional view of the amplitude of these electric and magnetic components in z-direction for TM and TE modes at Γ and K points are shown in figures 12 and at L, U, W and X points in figure 13 using finite difference time domain method using OptiFDTD [17].

In figure 14 the propagation of E_z and H_z in x-y plane in TM and TE modes through the fcc crystal formed from GaP spheres of radius $R=0.2a$ at Γ point of the Brillouin zone is presented. The amplitude of the electric field around the dielectric spheres is greater than the electric field inside the dielectric spheres. The electric field will not propagate through the dielectric spheres. But as the amplitude of the magnetic field (H) inside the spheres is higher than that of the outside the magnetic field will propagate through the dielectric avoiding propagation through air.

Fig. 13: The 3D view of the propagation variation of amplitudes of (a) E_z and (b) H_z for TM and TE modes at L , U , W and X points in GaP FCC photonic lattice with a filling factor of 0.134

Fig. 14: The propagation variation of amplitudes of (a) E_z and (b) H_z for TM and TE modes in x-y plane at the Γ point in GaP FCC photonic lattice with a filling factor of 0.134

6. Conclusions

For the fcc structures constructed with air spheres as localized medium with the dielectrics GaP, Si, InP, GaAs, InAs and Ge and BaSrTiO₃ as the background medium, there were only partial band gaps. The materials with smaller dielectric constants did not give any kind of a band gaps, but distorted the symmetry of the band diagrams. There was no complete band gap for SiO₂ ($\epsilon = 3.9$) spheres drilled in air for the filling factor in the range 0.017–0.740. For GaP, Si, InP, GaAs, InAs and Ge dielectrics spheres of radius $0.2a$ with filling factor 0.134 and for BaSrTiO₃ spheres of radius $0.3a$ with a filling factor of 0.452 in air, a complete band gap was obtained between second and third bands with a gap to mid gap frequency ratio in the range 3.59–5.37%. GaAs has nearly a constant band gap of $0.0181\omega a / 2\pi c$ in the range of spherical radius $r = (0.15 - 0.25)a$ and filling factor 0.0565–0.2618. GaP, Si, InP, GaAs, InAs and Ge gives the maximum band gaps for filling factor in the region 0.134. For dielectric spheres of $r = 0.15a$ with the filling factor is 0.0565 GaAs and InAs with dielectric contrast of 13.1 and 14.6 respectively give approximately same gap to mid gap ratio of 2.82% while for $r = 0.2a$ with filling factors of 0.134 and larger gap to mid gap ratio of 5.37% is obtained for GaP with dielectric contrast of 11.1. For $r = 0.25a$ with the filling factor of 0.262, the maximum mid gap ratio of 4.73% is obtained for InP with dielectric contrast of 12.4. In the dielectric contrast range 11–16 except for GaAs ($\epsilon = 13.1$) the largest gap to mid gap ratio was obtained with $r = 0.2a$ while for GaAs highest gap to mid gap ratio can be obtained with spheres of radius $r = 0.25a$. For telecommunication wave length of $1.55\mu\text{m}$, the largest band gap of 0.0292 normalized frequency was obtained for GaP for filling factor of 0.134 indicating that GaP dielectric spheres with radius $0.168\mu\text{m}$ in air is the most suitable fcc photonic crystal in this case. BaSrTiO₃ ($\epsilon = 200$) with a filling factor of 0.4524 can be used in microwave applications. Mode field distributions at symmetric points of GaP for telecommunication wavelength showed the occurrence of strong localization of the magnetic field within the sphere volume whereas the electric field spread over the spheres well into the surrounding air.

References

- [1] J.D. Joannopolus et al., Photonic Crystals: Modeling the flow of light, Princeton University Press, 2008, pp. 94-121.
- [2] E. Yablonovitch, T.J. Gmitter, Photonic band structure: the face-centered-cubic case, J. Opt. Soc. Am. A. 7 (9) (1990) 1792-1800.
- [3] J.W.S. Rayleigh, On the remarkable phenomenon of crystalline reflexion described by Prof. Stokes, Phil. Mag. 26 (1988) 256-265.
- [4] E. Yablonovitch, Inhibited spontaneous emission in solid-state physics and electronics, Phys. Rev. Lett. 58 (1987) 2059-2063.
- [5] K.M. Ho, C.T. Chan, C.M. Soukoulis, Existence of a photonic gap in periodic dielectric structures, Phys. Rev. Lett. 65 (1990) 3152-3155.
- [6] M. Maldovan, E. L. Thomas, Photonic crystals: six connected dielectric networks with simple cubic symmetry, J. Opt. Soc. Am. B. 22 (2005) 466-473.
- [7] S. John, Strong localization of photons in certain disordered dielectric superlattices, Phys. Rev. Lett. 58 (1987) 2486-2489.
- [8] E. Yablonovitch, T.J. Gmitter, Photonic band structure: The face-centered-cubic case Phys. Rev. Lett. 63 (1989) 1950.
- [9] K.M. Leung, Y.F. Liu, Full vector wave calculation of photonic band structures in face-centered-cubic dielectric media, Phys. Rev. Lett. 65 (1990) 2646.
- [10] Z. Zhang, S. Satpathy, Electromagnetic wave propagation in periodic structures: Bloch wave solution of Maxwell's equations, Phys. Rev. Lett. 65 (1990) 2650-2653.
- [11] H.S. Sözüer, J.W. Haus, R. Inguva, Photonic bands: Convergence problems with the plane-wave method, Phys. Rev. B. 45(24) (1992) 13962.
- [12] T. Suzuki, P.K. Yu, Tunneling in photonic band structures, J. Opt. Soc. Am. B. 12(5) (1995) 804-820.
- [13] R. Biswas et al., Photonic band gaps in colloidal systems, Phys. Rev. B. 57 (1998) 3701.
- [14] A. Moroz, C. Sommers, Photonic band gaps of three-dimensional face-centred cubic lattices, J. Phys.: Condens. Matter. 11 (1999) 997-1008.
- [15] K.B.S.K.B. Jayawardana, K.A.I.L. Wijewardena Gamalath, Body centered photonic crystal, Int. Lett. Chem. Phys. Astron. 66 (2016) 96-108.
- [16] K. Bethe, F. Welz, Preparation and properties of (Ba,Sr)TiO₃ single-crystals, Mater. Res. Bull. 6(4) (1971) 209-21.
- [17] OptiFDTD software package, Available at <https://optiwave.com/resources/academia/free-fdtd-download/>.