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Three dimensional photonic crystals

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ABSTRACT

The plane wave expansion method was implemented in modelling and simulating the band structures of three dimensional photonic crystals with FCC lattice formed from air spheres drilled in GaAs and diamond lattice formed by GaAs spheres drilled in air. Both these structures lead to a complete band gap not allowing EM waves with the frequency of the band gap to propagate through the crystal in any direction. Diamond lattice photonic crystal has a complete band gap for a wider range of filling fraction than FCC photonic crystal and also it has a wider band gap width.

***Keywords*:** Photonic crystal; plane wave expansion; GaAs, dielectric contrast; filling fraction; Fcc lattice and diamond lattice

1. INTRODUCTION

The three dimensional photonic crystals, an ideal three-dimensionally periodic structure (Figure 1) with a full band-gap in three-dimensions can be used in novel applications like band gaps, resonant cavities, wave guides etc. Unlike two dimensional photonic crystals, three dimensional photonic crystals have the freedom of controlling light in all along the three axes. But the band structures of these crystals are very complex and hard to predict. Manufacturing three dimensional photonic crystals is not easy and scientists are carrying giant researches to discover the means to facilitate the manufacturing process.

These photonic crystals are characterized by a periodic modulation of their dielectric constant in three spatial dimensions on a length-scale in the order of the wavelength of light they are intended to manipulate.

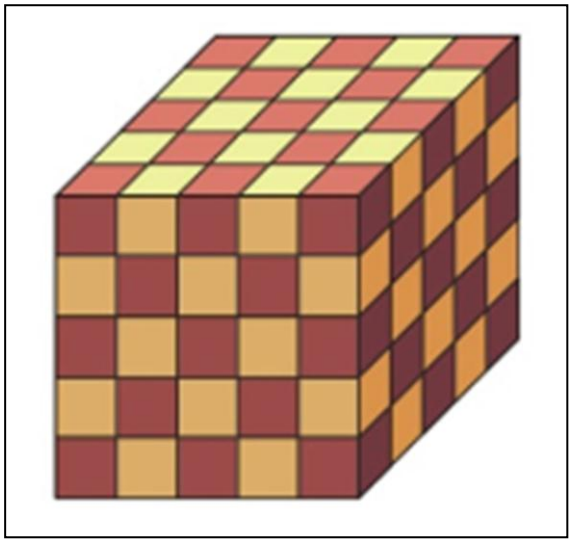


Figure 1. 3D Photonic Crystals.

This periodic variation of dielectric constant is achieved using a structure formed from two materials, typically a dielectric and air. The waves scatter from the periodic structure much like x-rays scattering from atoms within a crystalline solid. The periodic nature of the crystal leads to coherent scattering for certain directions as determined by the particular crystal symmetry, with an intensity that is dependent upon the constituent material properties [1]. The dispersion relation or band structure is used to analyze the properties of photonic crystals and determine whether photonic band gaps or pseudo photonic band gaps in a three dimensional photonic crystal that exist for some directions but not all, are present.

In 1987 Yablonovitch [2] and John [3] predicted the existence of the photonic band gap as well as the potential for inhibiting spontaneous emission and localizing light within defects in a periodic lattice of appropriate dimensions.

The first complete photonic band gap was achieved by Yablonovitch et al. in 1991 for the microwave regime [4]. By means of iterative optimization of approximate initial solutions through a parallel computing approach via block matrix diagonalization, Johnson and Joannopoulos [5,6] reduced the computational difficulty. As theoretical understanding and computational methods to calculate photonic band structure improved, researchers were guided to new structures, resulting in the demonstration of a complete photonic band gap in the NIR wavelengths.

In photonic band gap materials, the formation of photonic band gap is a result of macroscopic Bragg scattering and the microscopic Mie scattering. Scattering related to periodicity or the geometry of the lattice is Bragg scattering while the shape of individual scatterers are related to Mie scattering. The main parameter that affects the strength of these two scattering mechanisms is the refractive index contrast.

The effect is complex and hence there exist no simple correlation between the band gap and the parameters of photonic band gap structures. As a consequence, numerical calculations play a vital role in predicting the properties of light in these structures.

The periodic nature of photonic crystals makes plane wave expansion method well suited for calculations [7]. There are a number of computational implementations of this method for arbitrary structures [5,6].

The plane wave expansion method was adopted by Skoda [8] to compute the diffraction of two dimensional periodic band gap materials with finite thickness. Using this method Ho et al. [9] predicted the existence of complete band gap for a diamond lattice of spheres and established its dependence on dielectric contrast and filling fraction. The finite-difference time-domain method of computational analysis for electromagnetic systems allows for calculation of the time-evolution of electric fields in a given medium [10].

The calculations are performed by dividing the computation cell into discrete points and solving Maxwell's equations at each point in discrete time steps. This is, of course, an approximation of the real system which is improved as the discrete units of space and time are made smaller until a highly accurate representation of the true electromagnetic response may be calculated.

The plane wave expansion method applicable to any type of non-dispersive dielectric functions applied by us to two dimensional photonic crystals [11] was extended to three dimensions and used as the numerical technique in the present work in modelling and simulating the band structures of photonic crystals with FCC lattice formed from air spheres drilled in GaAs and diamond lattice formed by GaAs spheres drilled in air.

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 two lattice geometries. The effects of the parameters on the band gaps were studied.

2. PLANE WAVE EXPANSION

The propagation of light in a photonic crystal governed by Maxwell equations leads to the master equation for a periodic dielectric structure in terms of electric field $\boldsymbol{E}$ and magnetic field strength $\boldsymbol{H}$ with angular frequency ω:

$$\nabla \times \frac{1}{\varepsilon(r)} \nabla \times \boldsymbol{H} = \frac{\omega^2}{c^2} \boldsymbol{H}(r) \qquad (1)$$

Here photonic crystal was considered to be a macroscopic, homogeneous, isotropic dielectric material with no placed charges or current densities with real dielectric constant $\varepsilon(\boldsymbol{r})$ and no dispersion.

One of the most commonly used techniques for calculation of semiconductor band structure is the plane wave expansion method. A set of plane waves may be used to expand any function in a Fourier series given a periodic nature of the function.

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 $\boldsymbol{G}_i = h_i \boldsymbol{b}_i$ in terms of basis vectors in the reciprocal space $\boldsymbol{b}_i$ and set of are integers h_i,

$$\boldsymbol{H}(\mathrm{r}) = \sum_{\boldsymbol{G}_i,\lambda} h(\boldsymbol{G}_i,\lambda)\hat{e}_\lambda e^{i(\boldsymbol{k}+\boldsymbol{G}).\boldsymbol{r}} \qquad (2)$$

where $\hat{e}_\lambda$ are two orthogonal unit vectors perpendicular to $\boldsymbol{k}+\boldsymbol{G}_i$. The dielectric function of the structure is similarly expanded in terms of reciprocal lattice vectors.

$$\varepsilon(\boldsymbol{r}) = \sum_{G_i} \varepsilon(\boldsymbol{G}_i) e^{i\boldsymbol{G}\cdot\boldsymbol{r}}, \qquad \varepsilon(\boldsymbol{G}) = \int_A \varepsilon(\boldsymbol{r}) e^{-i\boldsymbol{G}\cdot\boldsymbol{r}} d^2 r \qquad (3)$$

The Fourier component $\varepsilon(\boldsymbol{G}-\boldsymbol{G}')$ is calculated by integrating over the area A of one lattice unit cell. Periodic dielectric function in real space can be simplified. Fourier transformation of the dielectric function can be further simplified to,

$$\begin{aligned} \varepsilon(\boldsymbol{G}) &= f\varepsilon_a + (1-f)\varepsilon_b \quad \text{for } \boldsymbol{G}=0 \\ &= (\varepsilon_a - \varepsilon_b) S(\boldsymbol{G}) \quad \text{for } \boldsymbol{G}\neq 0 \end{aligned} \qquad (4)$$

where ε_a and ε_b refer to the dielectric constants of the localized medium and background respectively and f is the filling factor, defined as the fraction of area occupied by the localized medium in one unit cell. The factor $S(\boldsymbol{G})$ relying on the geometry of the localized medium and the lattice structures is given by,

$$S(\boldsymbol{G}) = \frac{1}{A}\int_{A_d} e^{-i\boldsymbol{G}\cdot\boldsymbol{r}} d^2 r \ . \qquad (5)$$

The structure factor for a three dimensional sphere with radius R is given by

$$S(G) = 3f\left[\frac{\sin(GR) - GR\cos(GR)}{(GR)^3}\right] \qquad (6)$$

Substituting equations 2 and 3 in 1:

$$\sum_{G'} |\vec{k}+\vec{G}||\vec{k}+\vec{G'}|\,\varepsilon^{-1}(\vec{G}-\vec{G'}) \begin{bmatrix} \hat{e}_2.\hat{e}'_2 & -\hat{e}_2.\hat{e}'_1 \\ -\hat{e}_1.\hat{e}'_2 & \hat{e}_1.\hat{e}'_1 \end{bmatrix} \begin{bmatrix} h'_1 \\ h'_2 \end{bmatrix} = \begin{bmatrix} M_1 & M_2 \\ M_3 & M_4 \end{bmatrix} \begin{bmatrix} h_1(G') \\ h_2(G') \end{bmatrix} = \frac{\varpi^2}{c^2} \begin{bmatrix} h_1 \\ h_2 \end{bmatrix} \qquad (7)$$

Unlike in one dimensional and two dimensional simplifications, master eigenvalue equation does not exist in three dimensional case. Hence the two unit vectors $\hat{e}_{1,k+G}$ and $\hat{e}_{2,k+G}$

which are perpendicular to $k + G$ vector, had to be calculated. First, grid points in space were specified in a three dimensional grid.

Number of grid points or plane waves used was $(2n+1)^3$, where n is the number of grid points in the direction of each basis lattice vectors. Hence the complexity and dimensions of dielectric function would be so large compared to two dimensional photonic crystals. In this study, only the dielectric spheres were considered as the localized medium.

The analytical expression for calculating Fourier transform of a sphere was used in both cases. After specifying the high symmetrical points in a three dimensional geometry, all the coefficients in matrix M were formed by calculating two unit vectors. All the eigenvalues for the matrix were calculated for each k vector in the first irreducible Brillouin zone.

3. FCC CRYSTAL LATTICE

The face-centered cubic lattice (FCC) and the Brillouin zone, which is the Wigner–Seitz primitive cell in the reciprocal lattice is shown in Figure 2.

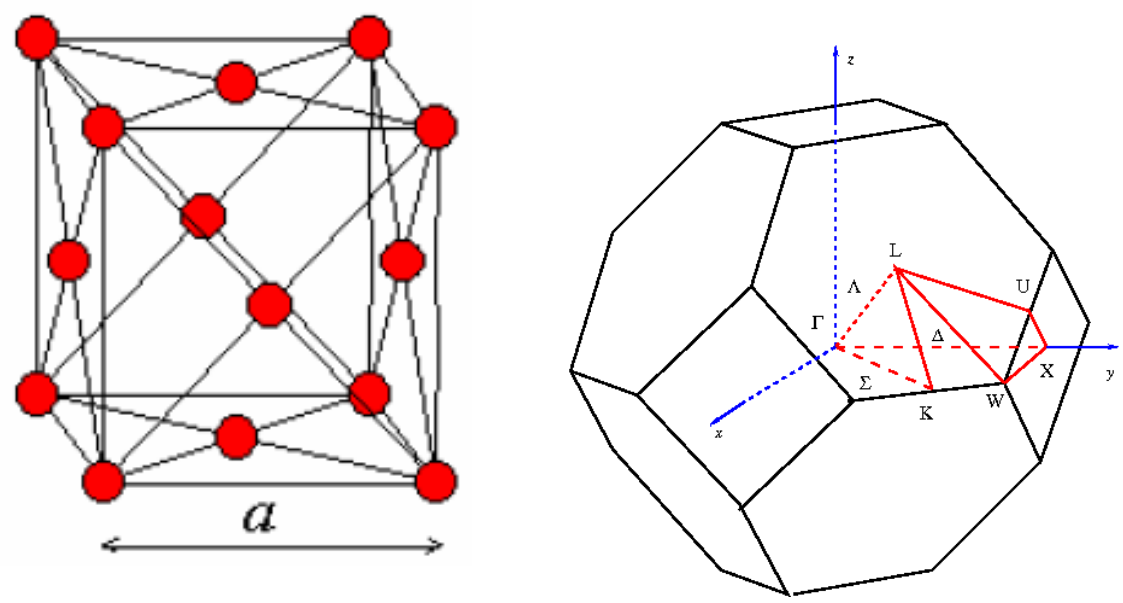


Figure 2. FCC lattice (left) and the first Brillouin zone (right).

There is one host atom at each corner and one host atom in each face in the unit cell. Basis lattice vectors are $\boldsymbol{a}_1 = (0,1,1)\,a/2$, $\boldsymbol{a}_2 = (1,0,1)\,a/2$ and $\boldsymbol{a}_3 = (1,1,0)\,a/2$ with atom positions $(0,0,0)a$.

Basis reciprocal lattice vectors are $\boldsymbol{b}_1 = 2\pi(-1,1,1)/a$, $\boldsymbol{b}_2 = 2\pi(1,-1,1)/a$ and $\boldsymbol{b}_3 = 2\pi(1,1,-1)/a$. For a photonic crystal with a FCC lattice formed by air holes drilled in

GaAs, with a dielectric constant $\varepsilon = 13$, the band diagram with modified frequency $\omega a / 2\pi c$ verses wave vector is shown in Figure 3.

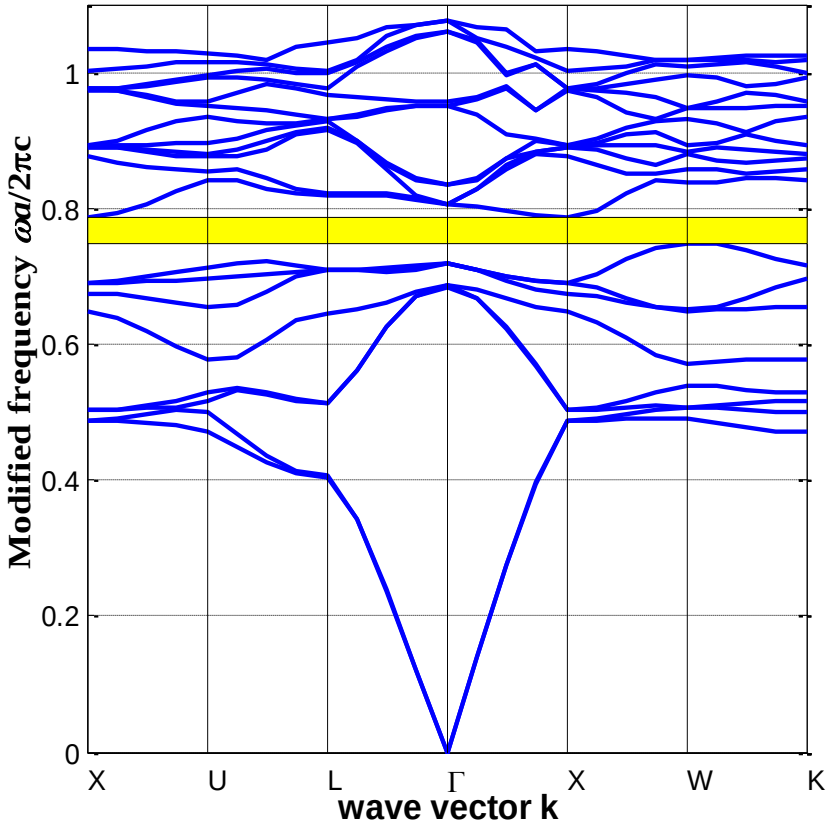


Figure 3. The band structure of three dimensional FCC lattice with air holes drilled in a GaAs medium with ε_b =13

The filling fraction considered is 0.74 of the closed packed filling fraction of FCC lattice. The complete band gap, highlighted in yellow occurs between the eighth band and ninth band. Band gap width is about 0.0384 $(\omega a/2\pi c)$ and gap to mid gap ratio is 5%. The band gap occurred in high frequency region. The structure can be used in applications at telecommunication wavelength. For instance, in order to create a structure operating around $\lambda = 1.55\,\mu\text{m}$, from the mid-gap frequency 0.7682$(\omega a/2\pi c)$ lattice constant *a* is 1.1907 μm and the radius of the holes must be 0.4210 μm.

The band structure of the photonic crystal not only describes the presence of photonic band gap, it also lends insight into light propagation within the crystal, specifically the group velocity of light as it travels through the photonic crystal. Flat bands seen in the high energy regions of the band structure and near the edges of the Brillouin Zone at the high symmetry points shown in the figure are indicative of low group velocities.

The band structure relates the frequency and wave vector and therefore to the group velocity of light.

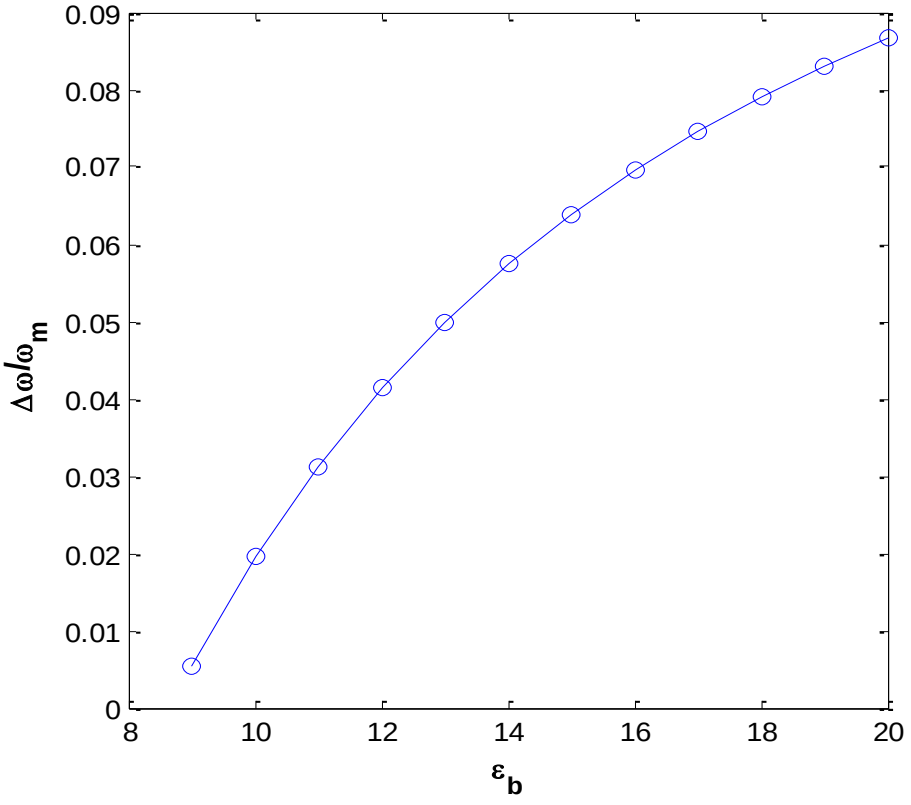
This is particularly useful if materials that rely on light-matter interaction, such as nonlinear optical materials are incorporated into the photonic crystal as their properties should be enhanced due to the low group velocity.

The scattering strength in the crystal may be assessed qualitatively by the refractive index contrast between the two materials, specifically the ratio of their refractive indices. The existence and size of a photonic band gap in a photonic crystal depend on the symmetry of the crystal and the magnitude of the difference in refractive index between the materials in the system. Therefore for each crystal structure there is a minimum refractive index contrast, which opens a photonic band gap. In order to increase the size of the gap, the difference in refractive index should be maximized.

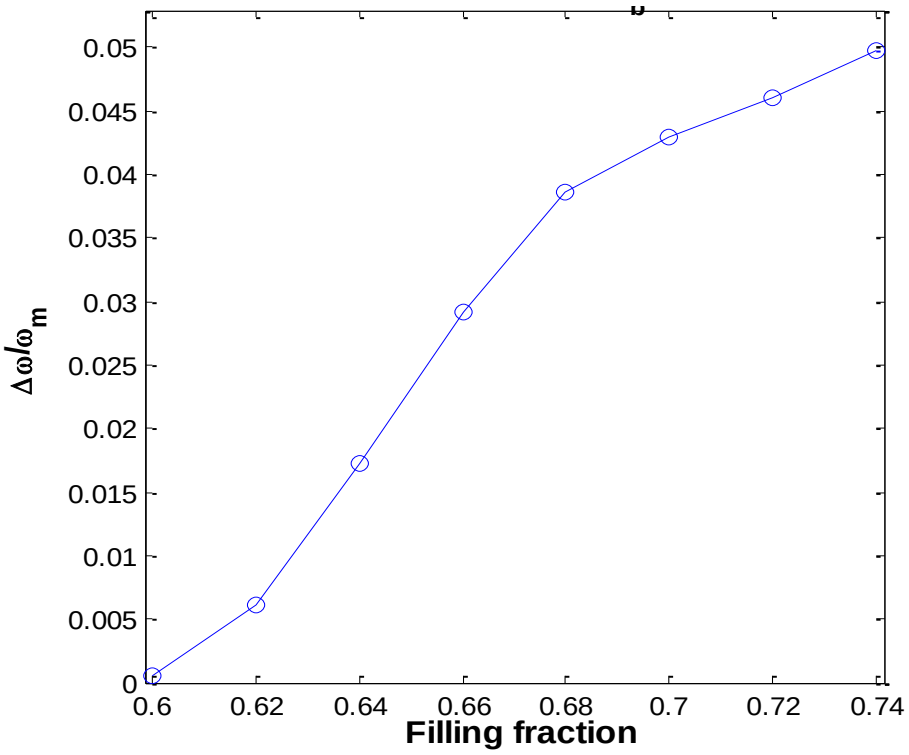
The variation of gap width to mid gap ratio of the FCC lattice with dielectric contrast and filling fraction are presented in Figure 4.

The gap width to mid gap ratio was increased with dielectric constant ε_b .

The figure 3(*a*) also reveals the minimum dielectric constant ε_b or the minimum dielectric contrast to open a complete band gap is 9. Hence the background materials having a dielectric constant below 9 will not have a complete band gap. The variation of gap width to mid gap ratio with filling fraction shows that the closed packed filling fraction 0.74, yields the largest gap. The gap width decreases when the filling fraction reduces. Also a minimum filling fraction of 0.6 and the minimum filling fraction needed to have a complete band gap is 0.6.



3(*a*)



3(*b*)

Figure 4. The variation of gap to mid gap ratio of 3D FCC photonic crystal with air spheres in a dielectric medium with ε_b=13. (a) variation with ε_b (b) *V*ariation with filling fraction

4. DIAMOND CRYSTAL LATTICE

The space lattice of a diamond is a face–centered cubic with two spherical atoms in the unit cell as shown in Figure 5.

Assuming the length of the simple cubic side is *a*, the primitive lattice vectors are $\boldsymbol{a}_1 = (0,1,1)a/2$, $\boldsymbol{a}_2 = (1,0,1)a/2$ and $\boldsymbol{a}_3 = (1,1,0)a/2$, with atom positions $(0,0,0)a$ and $(1/4,1/4,1/4)a$.

Basis reciprocal lattice vectors are $\boldsymbol{b} = (-1,1,1)2\pi/a$, $\boldsymbol{b}_2 = (1,-1,1)2\pi/a$ and $\boldsymbol{b}_3 = (1,1,-1)2\pi/a$.

The Brillouin zone, which is the Wigner–Seitz primitive cell in the reciprocal lattice is also shown in the Figure 5 (right).

Assuming the radius of the sphere is *R*, the Fourier coefficient at the reciprocal lattice grid was expressed using the shift property of Fourier transform and the analytical expression of a sphere Assuming the radius of the sphere is *R*, the Fourier coefficient at the reciprocal lattice grid was expressed using the shift property of Fourier transform and the analytical expression of a sphere is

$$S(\boldsymbol{G}) = 3f\left[\frac{\sin(\boldsymbol{G}\cdot\boldsymbol{R})-\boldsymbol{G}\cdot\boldsymbol{R}\cos(\boldsymbol{G}\cdot\boldsymbol{R})}{(\boldsymbol{G}\cdot\boldsymbol{R})^3}\right]\cos(\boldsymbol{G}\cdot\boldsymbol{r}_0) \quad (8)$$

where $\boldsymbol{r}_0$ is equal to $(1/4,1/4,1/4)$. The filling fraction f is

$$f = 2\times\frac{4\pi R^3}{3a^3} \quad (9)$$

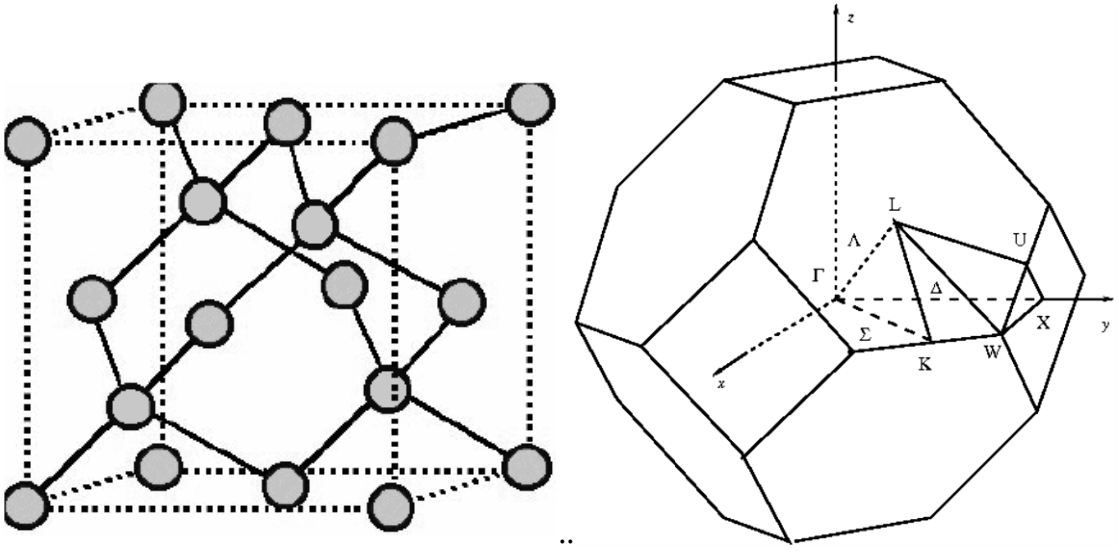


Figure 5. Diamond lattice (left) and the first Brillouin zone (right).

The band structure for 3D diamond lattice with GaAs dielectric spheres with ε = 13 drilled in air is shown in Figure 6.

This structure has a large complete band gap $0.433-0.503\,(\omega a/2\pi c)$ between second and third bands. Variation of gap to mid gap frequency with dielectric contrast and filling factor is presented in Figure 7. As expected, the gap width increased with dielectric contrast and also with filling factor.

The minimum dielectric contrast needed to open a complete band gap was around $\varepsilon = 4.1$. The maximum band gap occurred for close packed condition of Diamond lattice, when the filling fraction was equal to 0.34.

The main difference between this structure and FCC lattice was; this structure has a complete band gap in a wider range of filling fractions.

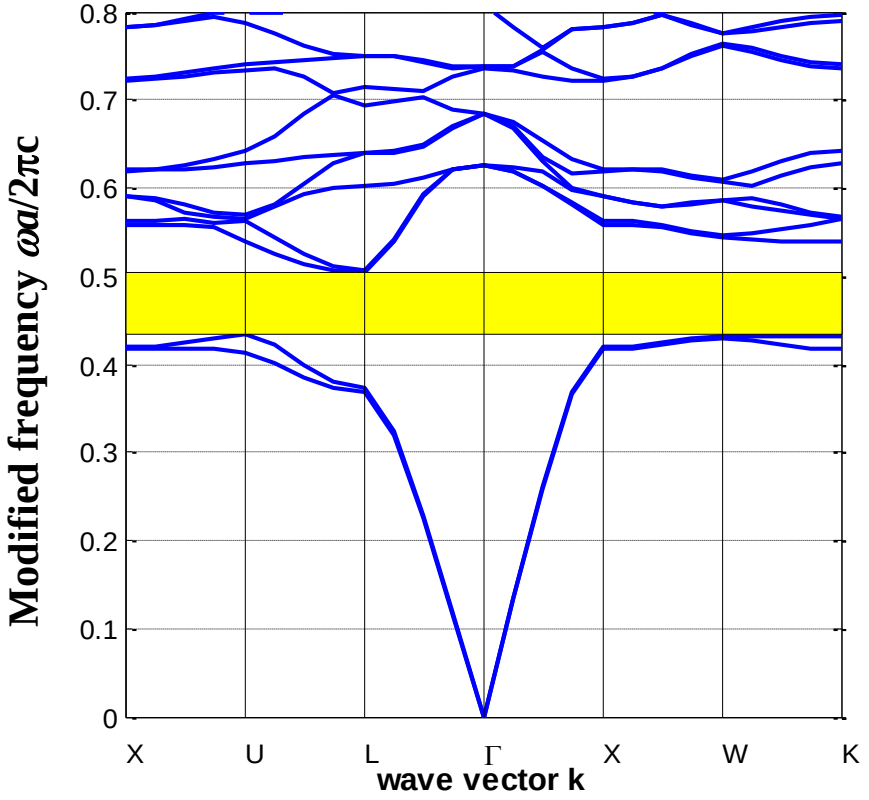
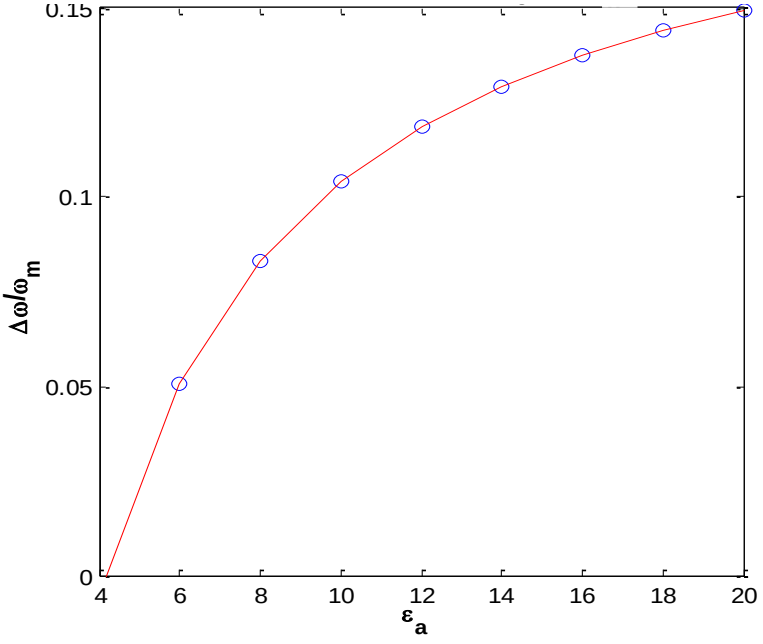
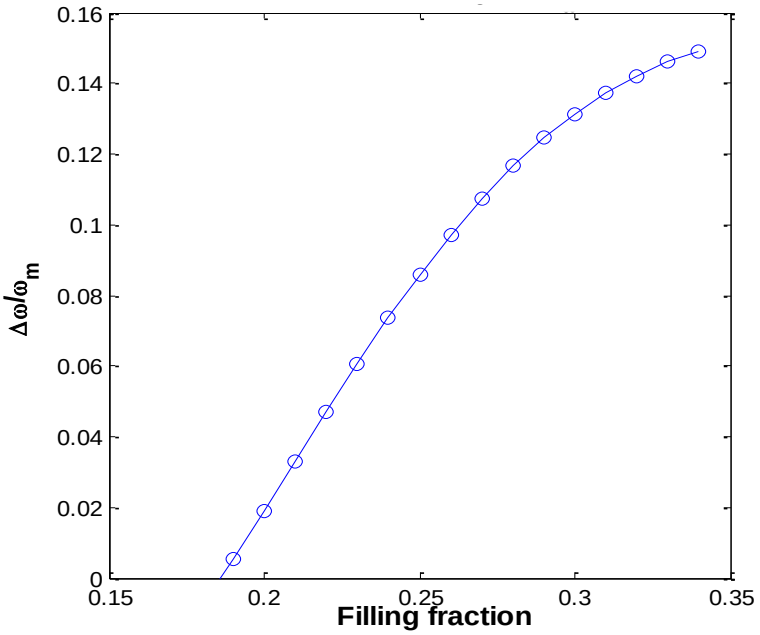


Figure 6. The band structure of three dimensional diamond lattice formed from GaAs spheres drilled in air ε_a =13.



6(*a*)



6(*b*)

Figure 7. The variation of gap to mid gap ratio of 3D diamond photonic crystal formed from GaAs spheres in air ε_a =13. (a) variation with ε_a (b) *V*ariation with filling fraction.

5. CONCLUSIONS

The band diagram for three dimensional face centred cubic photonic lattice formed from air spheres drilled in GaAs dielectric medium gave a complete band gap of 0.0384 $(\omega a/2\pi c)$ with a gap to mid gap ratio 5%. This structure with a lattice constant 1.1907 μm formed from air spheres of radius 0.4210 μm drilled in GaAs can be used to operate at telecommunication wavelength $\lambda = 1.55\,\mu m$. The minimum dielectric contrast of 9 and minimum filling fraction of 0.6 are needed to open a complete band gap. For the diamond photonic lattice formed from GaAs dielectric spheres drilled in air gave a much larger band gap of 0.07 $(\omega a/2\pi c)$. Also a complete band gap could be obtained for wider range of filling fractions. The minimum dielectric contrast of 4.1 and minimum filling fraction of 0.18 were needed to open a complete band gap. For both lattices the maximum band gap occurred for close packed condition.

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