

# Variation of Single waveguide modes with dielectric constant of line defect in 2D Photonic Crystals of dielectric rods in air: A Simulation based analysis

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## Abstract

*It is observed that a 2D Photonic crystal model of dielectric rods in air in square and triangular lattice configurations have a complete band gap in TM mode. A line defect created by making the radius of the rods along a line half of the normal case creates a waveguide with a single waveguide mode in the band gap region. In this paper the variation in the relevant features of this single mode with dielectric constant of the line defect has been explored by simulation method.*

## 1. Introduction

Photonic crystals are dielectric material structures based on periodic modulation of dielectric constant. They find numerous optical applications. The periodic variation of dielectric constant may be along a line as 1D, in a plane as 2D and in space as 3D respectively.

Photonic crystal structure medium responds to an electromagnetic wave by determining its wavelength and direction of propagation. This is suitably described by the dispersion relation associating frequency of the wave with the wave vector it assumes in the medium. Remarkably, the behaviour in unit domain or region of periodicity is repeated everywhere in the medium both in terms of structural as well as functional features. Hence dispersion relation in this unit region completely describes itself for the entire medium. This gives rise to Band structure and the region in inverse space coordinates (to match the dimension of the wave vector) is the first Brillouin zone.

Suitable structural modulation can achieve the desired propagation features in the medium and even provide for Band gap i.e the range of frequency for which light cannot propagate through the medium. Photonic crystals are used on millimetre periodic scale for microwave range applications and on micro or nano metre scale for optical range of electromagnetic waves.

A 2D photonic crystal has refractive index variation in a 2D plane, where as in the direction normal to this the refractive index remains constant. Common examples of 2D photonic crystals are square and triangular lattice of dielectric rods embedded in background material of lower dielectric constant and triangular lattice of air holes in dielectric slab. Suitable modification in this periodic refractive index pattern provides desired control over the behaviour and propagation of light.

## 2. Theory

The photonic crystals with series of point defects and line defects can be used as waveguides with their own modes.

The band structures of 2D photonic crystals with line defect for both square lattice and triangular lattice structures have been computed by using PWEM method. The band structure is the dispersion relation between the frequency of the electromagnetic wave and the wavevector  $k$  it assumes inside the crystal medium. A real  $k$ -number indicates that the particular frequency is allowed inside the medium. An imaginary  $k$ -number indicates that the particular frequency is not allowed. This dispersion relation is obtained by solving the following master equation

$$\nabla \times \left( \frac{1}{\epsilon(\mathbf{r})} \nabla \times \vec{H}(\mathbf{r}) \right) = \left( \frac{\omega}{c} \right)^2 \vec{H}(\mathbf{r}) \quad (1)$$

The above equation is derived from the two curl equations from the set of Maxwell equations for dielectric media.

In this equation,  $\epsilon(\mathbf{r})$  is the periodic dielectric function; as such the Bloch periodicity theorem is applied for the periodic dielectric constant variation and due to that electromagnetic field distribution in the medium is also periodic.

In the above equation  $\vec{H}(\mathbf{r})$  is the magnetic distribution which is periodic,  $\omega$  represents the frequency of permissible mode and it is calculated as  $\omega_{k,n}$ , where  $k$

is the wave vector of the medium and  $n$  is the  $n$ th frequency value ( $n$ th mode) associated with that  $k$ .

In this paper the numerical method we have used for analysis is Plane Wave Expansion Method (PWEM) which is a frequency domain technique based on Bloch's theorem of periodicity. It consists of expanding both the periodic dielectric functions and electromagnetic field solution in infinite series of uniform plane waves and thus reducing the Boundary Value Problems (BVP) to a set of Eigen value equations.

Photonic Band Gap structures are scalable in terms of the period of the lattice. As such, the parameters describing their features are conveniently expressed as normalised quantities i.e. in dimension less units. They can be expressed in relevant physical units by multiplying them with the corresponding conversion factor.

For the band structure  $k$ -points are sampled from the first Brillouin zone of the respective lattice structure which can further be reduced to the points on the contour of irreducible Brillouin zone.

## 2. Design of the lattices with line defect

In this paper we consider the 2D photonic crystal structures consisting of square and triangular lattice of dielectric rods in air. Line defects in both the structures have been created by reducing the radius of dielectric rods along one particular row to half the regular value and then varying the dielectric constant along that row as shown in Fig. 1.

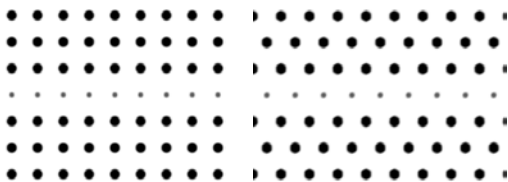


Figure 1. Square and triangular lattice configurations with Line defects respectively

Our structures are infinitely long rods in air in direction normal to the plane of periodicity, approximating that the modes are confined in periodic plane due to this infinite height. The periodicities of both square and triangular lattice structures are 1 each and the dielectric constant of the normal rods is 12.

For the square lattice case, the radius of normal rods is 0.19. The radius of defect rods is set to 0.095 and their

dielectric constant is varied between 1 and 16 in steps of one.

For the triangular lattice case, the radius of normal rods is 0.18. The radius of defect rods is set to 0.09 and their dielectric constant is varied between 1 and 16 in steps of one as before.

In integrated photonic circuits this line defect serves as the waveguide.

## 3. Band structure of square and triangular lattice structures with line defect

For the band structure concerning the line defect the  $k$ -points have been sampled along  $\Gamma X$  direction in the square lattice structure and  $\Gamma K$  direction in the triangular lattice structure between 0 and 0.5 (normalized units) and interpolated with 15 equidistant points as shown in Fig. 2. The frequency is also normalized.

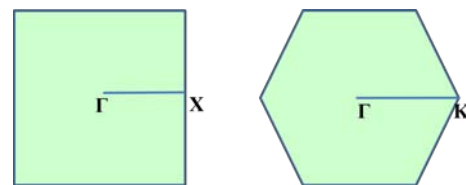


Figure 2. Brillouin Zones for square and triangular lattices with  $k$ -paths for line defect

The band structure for the line defect of the two lattice structures are shown below in Fig.3 and Fig.4. The red curve is the line defect mode and in integrated photonic circuits this represents the waveguide mode where this line defect serves as the waveguide.

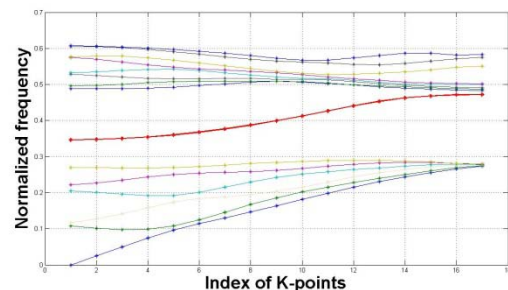


Figure 3. TM Band structure for square lattice with line defect

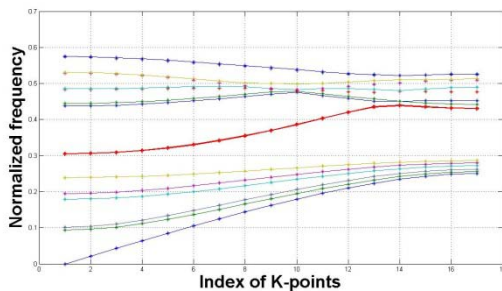


Figure 4. TM Band structure for triangular lattice with line defect

## 4. Parameters computed and analysed

### 4.1. Line Defect Mode

#### 4.1.1 Air mode, Dielectric mode and Line defect (waveguide) mode

The band structures for both square lattice and triangular lattice cases have been obtained with variation in index of k-points along the line defect. As shown in Fig. 3 and Fig. 4 these band structures have air modes (above the band gap region) and dielectric modes (below the band gap region) separated by a line defect mode of permissible frequencies in the band gap region, which is represented by the thick red curve in both square as well as triangular lattice band structures. To get the actual values of permissible frequencies and k-points we need to multiply frequency and k-point with  $\frac{2\pi c}{a}$  and  $\frac{2\pi}{a}$  respectively as conversion factor. Here 'a' stands for period of the lattice and 'c' is the speed of light in free space.

#### 4.1.2. Upper frequency limit

This is the maximum permissible frequency of the line defect mode (Waveguide mode). The variation of this parameter with defect dielectric constant has been plotted for both square lattice as well as triangular lattice structures as shown in Fig. 7.

#### 4.1.3. Lower frequency limit

This is the minimum permissible frequency of the line defect mode (Waveguide mode). The variation of this parameter with defect dielectric constant has been plotted for both square lattice as well as triangular lattice structures as shown in Fig. 8.

#### 4.1.4. Mid frequency

This is the average (arithmetic mean) of upper limit (maximum) and lower limits (minimum) permissible frequencies. This parameter has also been analysed by

varying defect dielectric constant for both square lattice as well as triangular lattice structures as shown in Fig. 9

### 4.1.5. Frequency span

This gives the interval of frequencies of the permissible line defect mode (Waveguide mode), which is the difference between Upper frequency limit and Lower frequency limit. The variation of frequency span with defect dielectric constant has been analysed for both square as well as triangular lattice structures as shown in Fig. 9.

### 4.1.6. Frequency span as a fraction of band gap

This gives the interval of frequencies in line defect mode (Waveguide mode) relative to band gap of photonic crystal without defect as ratio. The variation of this parameter with defect dielectric constant has been analysed for both square lattice as well as triangular lattice structures as shown in Fig. 10.

## 4.2. Group Velocity

The concept of group velocity is important for understanding light wave propagation and quantifying dispersion. It is the speed of the light pulse with a narrow frequency spread about central frequency. It is mathematically defined as  $\frac{d\omega}{dk}$ . In this paper group velocity variation at each k-point and also for each frequency value for both square lattice as well as triangular lattice have been shown for different defect dielectric constants. It has been expressed in the normalized unit and to get the actual value it needs to multiply with c, the velocity of light in free space.

## 4.3. Effective Refractive Index

This dimensionless parameter measures the resistance offered by the optical medium to electromagnetic wave propagation. As such it is measured as the ratio of velocity of light in free space to the velocity in that medium. It is function of frequency. For the line defect mode having the collection of continuous frequency values in its frequency span it can be expressed as the ratio of velocity of light in free space to the group velocity at the particular frequency and its k-point. i.e. it is inversely proportional to the group velocity of the medium. In this paper the variation of effective refractive index with k-point and with frequencies of the line defect mode has been analysed for different defect dielectric constants. As the group velocity has been expressed normalised so its inverse directly gives the effective index.

#### 4.4. Group Velocity Dispersion (GVD)

This parameter is also important to analyse dispersion of the propagation mode in its medium. It is mathematically defined as  $\frac{d^2\omega}{dk^2}$ . Here, we analyse GVD with the variation of k-point and defect mode frequencies for both square lattice as well as triangular lattice structures, for different defect dielectric constant values. A conversion factor of  $\frac{ac}{2\pi}$  has to be multiplied with the normalised values to express them in the relevant physical units.

#### 5. Computational Results

The line defect modes (waveguide modes) for both square lattice and triangular lattice structures have been obtained for different defect dielectric constants. The Upper frequency limit, Lower frequency limit, Frequency span, Frequency span as a fraction of band gap of the structure are extracted from waveguide mode characteristics for different defect dielectric constant values.

Group velocity and GVD variations have been plotted against k-points and frequencies for both square lattice and triangular lattice structures. These parameters are calculated by converting the differential equations into suitable difference equations.

In band structure diagrams of square lattice and triangular lattice structures with the line defect, the line defect modes are represented by thick red curves as against the thin and fading appearance of the air modes and dielectric modes as shown in Fig. 3 and Fig. 4. In the analysis the other parameters like group velocity, GVD and effective refractive index characteristics (corresponding to different defect dielectric constant values) are represented by curves of different colours. The values of the defect dielectric constants are also indicated on each plot.

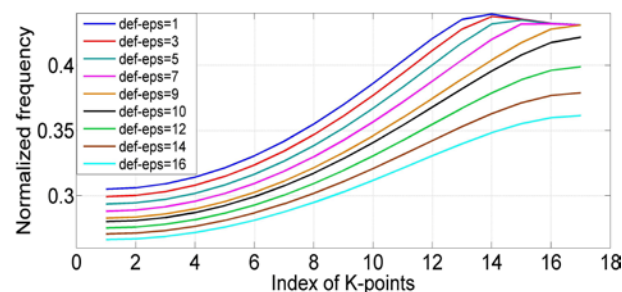


Figure 5. Single line defect modes for square lattice for different defect dielectric constants

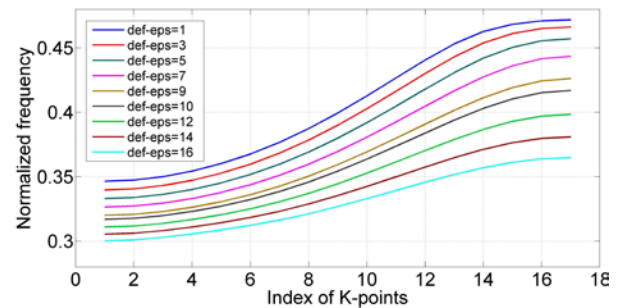


Figure 6. Single line defect modes for triangular lattice for different defect dielectric constants

We observe, in the case of square lattice and triangular lattice structures, with increase in defect dielectric constant the line defect modes are continuously moving downwards (decrease in frequency all k-points) towards dielectric modes.

This defect mode divides the band gap region into two parts. The upper region between the air mode and the defect mode with no allowed frequency mode in lattice increases with increase in defect dielectric constant. Similarly the lower region between the defect mode and the dielectric mode with no allowed frequency mode decreases with increase in defect dielectric constant.

For square lattice structure, there is overlap of frequencies of the waveguide modes for defect dielectric constant values of 1 to 9 as shown in Fig. 5. This happens at higher index of k-points. In this range of defect dielectric constant the group velocity ( $\frac{d\omega}{dk}$ ) becomes negative.

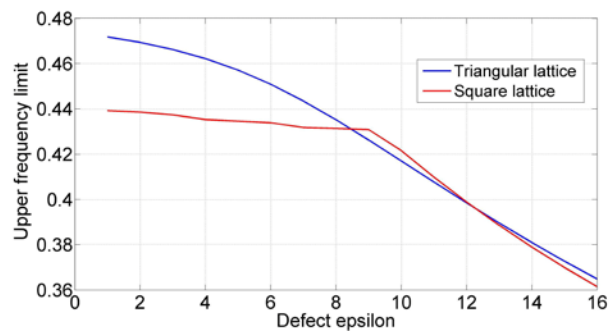
Unlike in the case of square lattice, in the case of triangular lattice the group velocity is positive for all k-points since the waveguide mode curves are non decreasing curves i.e. as the k-point is increased the permissible normalized frequency does not decrease as shown in Fig. 6.

The normalized frequency values vary from 0.25 to 0.44 for all these waveguide modes for unity period and they vary around 0.35 mid frequency value. Hence, for 0.5  $\mu\text{m}$  period they vary around 0.7 normalized value i.e. wavelength value lies around 3<sup>rd</sup> optical window of 1.55 $\mu\text{m}$ .

For triangular lattice structure the normalized frequency values vary from 0.3 to 0.48 for all waveguide for unity period and vary around 0.39

frequency value. Hence for  $0.5\mu\text{m}$  period they vary around 0.8 normalized values, i.e wavelength value lies around 2<sup>nd</sup> optical window of  $1.33\mu\text{m}$ .

**Frequency distribution of waveguide modes for different structures**

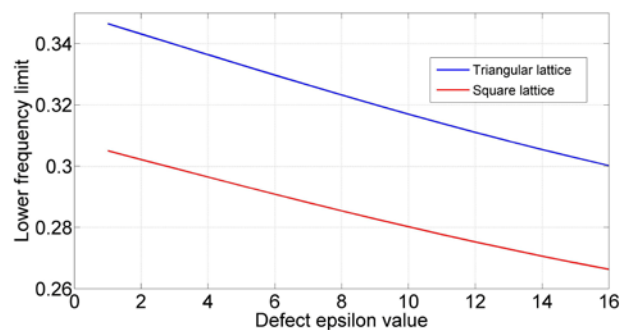


**Figure 7. Variation of Upper frequency limit against defect dielectric constant**

For triangular lattice the parameter Upper frequency limit decreases monotonically and smoothly with increase in defect dielectric constant and this decrease is almost linear between defect dielectric constant values 7 to 16 with slope of -0.0085 as shown in Fig. 7.

In case of triangular lattice the maximum value of Upper frequency limit i.e. 0.474 occurs at defect dielectric constant 1 and minimum value at dielectric constant 16, i.e. 0.365.

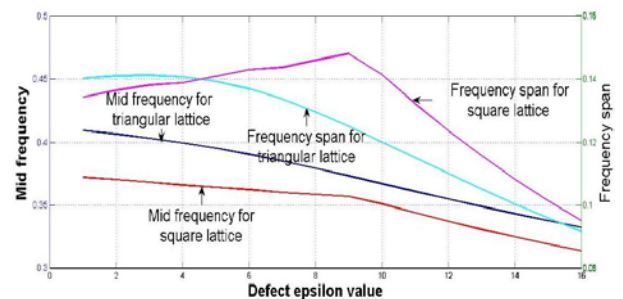
In case of square lattice, Upper frequency limit is monotonically decreasing with increase in defect dielectric constant. But at defect dielectric constant 9 there is sharp change in the decrease pattern. Between defect dielectric constant 9 and 16 this decrease is steep and almost linear with slope of -0.101 as shown in Fig. 7. It has maximum value at defect dielectric constant 1 i.e. 0.44(in normalized frequency unit) and minimum value at defect dielectric constant 16 i.e. 0.362.



**Figure 8. Variation of Lower frequency limit against defect dielectric constant**

In case of triangular lattice structure, Lower frequency limit is monotonically decreasing and this decrease is linear with slope of -0.003. The maximum value at defect dielectric constant value 1 is 0.347 and the minimum value at defect dielectric constant value 16 is 0.3 as shown in Fig. 8.

In case of square lattice structure, Lower frequency limit is approximately linear between defect dielectric constant values 1 and 16 with slope of -0.0027. The characteristics are similar to that of triangular lattice structure as shown in Fig. 8.



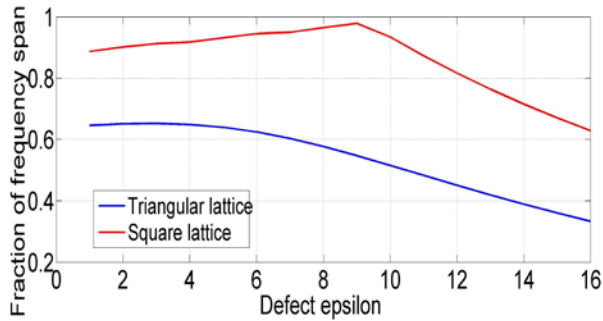
**Figure 9. Variation of Mid frequency and frequency span against defect dielectric constant**

In case of triangular lattice, frequency span characteristics are relatively flatter and it decreases monotonically with increase in defect dielectric constant. The curve is approximately linear between defect dielectric constant 6 and 16 with slope of -0.0055 as shown in Fig. 9.

In case of square lattice structure, frequency span characteristics increases monotonically between defect dielectric constants 1 and 9 and decreases almost linearly from defect dielectric constants 9 to 16 with slope of -0.0074 as shown in Fig. 9.

For triangular lattice structure, the parameter mid frequency decreases slowly between defect dielectric constant values 1 and 4 and there onwards decreases more rapidly as shown in Fig.9. The characteristics are almost linear between defect dielectric constants 6 and 16 with slope of -0.0058.

In case of square lattice structure, mid frequency shows irregular behaviour between defect dielectric constants 1 and 9. This is due to the nature of Upper frequency limit between defect dielectric constants 1 and 9. The curve is decreasing almost linearly between defect dielectric constants 9 and 16 with slope of -0.006 as shown in Fig.9.

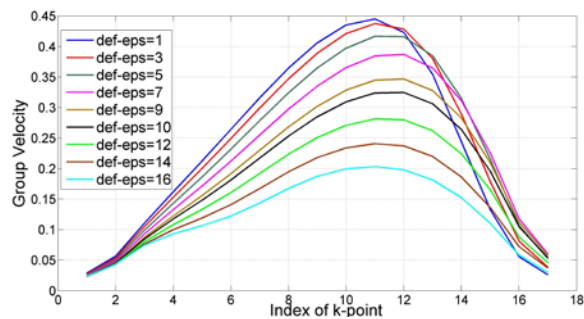


**Figure 10. Variation of fraction of frequency span against defect dielectric constant**

The parameter fraction of frequency span is simply normalized version of frequency span characteristics obtained. In case of triangular lattice structure it has maximum value 0.655 at defect dielectric constant 1 and minimum value 0.34 at dielectric constant 16 as shown in Fig. 10. In case of square lattice structure it has maximum value 0.97 at defect dielectric constant 9 and minimum value 0.64 at defect dielectric constant 16. Unlike triangular lattice square lattice waveguide modes utilise more of band gap.

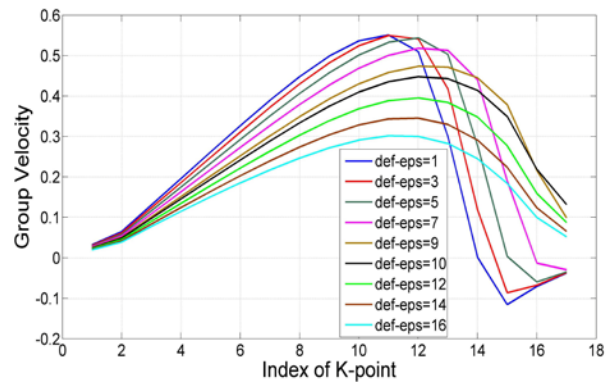
**Variation of Group Velocity with k-point:**

In case of triangular lattice structure group velocity monotonically increases up to k-point 11 or in some cases up to k-point 12 and then monotonically decreases i.e. the maxima lies at k-point 11 and 12. The monotonically increasing portion of these characteristics is relatively flatter and the decreasing portions are relatively steeper. The variation of group velocity with k-point is almost linear between k-points 3 and 9 for defect dielectric constant values 1 to 9. For defect dielectric constant 10 to 16 this variation is not linear as shown in Fig. 11.



**Figure 11. Variation of group velocity of triangular lattice structure against index of k-point for different defect dielectric constants**

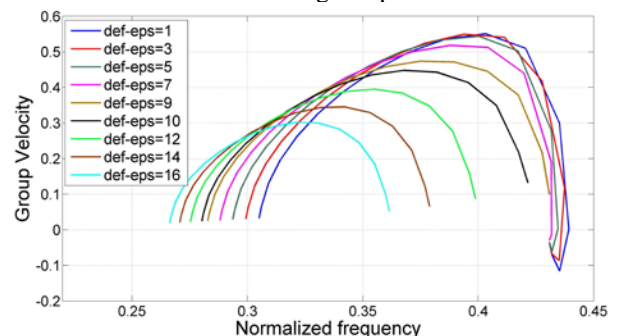
In case of square lattice structure similar behaviour is observed. But in this case negative group velocity is found for defect dielectric constant values 1, 3, 5, 7 corresponding to the region where waveguide modes overlap in frequency and they start decreasing there onwards, as shown in Fig. 12. The peak values of square lattice curves are always greater than those of triangular lattice curves for all defect dielectric constant.



**Figure 12. Variation of group velocity of square lattice structure against index of k-point for different defect dielectric constants**

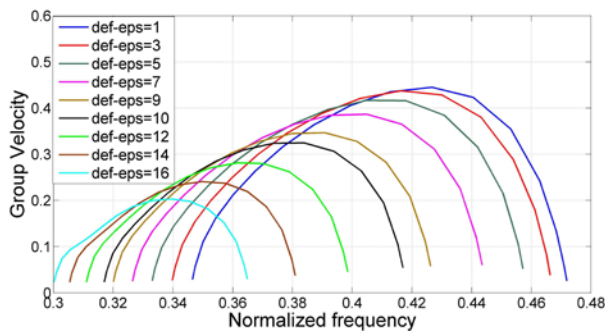
**Variation Group velocity with frequency:**

Group velocity in square lattice structure increases with frequency for a particular defect dielectric constant monotonically and reaches its respective maxima and then decreases monotonically (except for negative group velocity cases for dielectric constants 1,3,5); the rise being comparatively flatter and the fall being steeper as shown in Fig. 13. The maxima (maximum value) of all these group velocity curves decrease with defect dielectric constant i.e. the lowest defect dielectric constant has the highest peak value.



**Figure 13 Variation of group velocity of square lattice structure against normalized frequency for different defect dielectric constants**

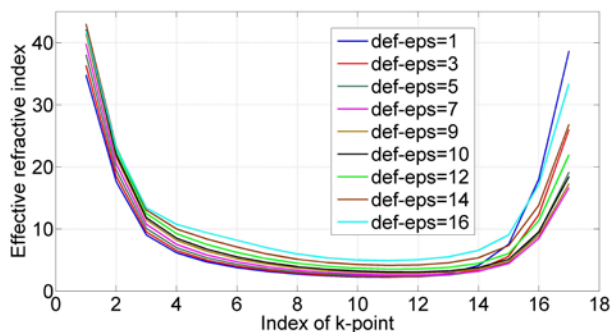
In case of triangular lattice structure group velocity curves monotonically increase till their respective maximum value and then monotonically decrease, where this decrease is relatively steeper. This is observed for all defect dielectric constant as shown in Fig. 14. The maximums of all these group velocities decrease with defect dielectric constant value. The behaviour here is similar to square lattice structure except that there are no negative group velocity values.



**Figure 14** Variation of group velocity of triangular lattice structure against normalized frequency for different defect dielectric constants

**Variation of Effective refractive index with k-point:**

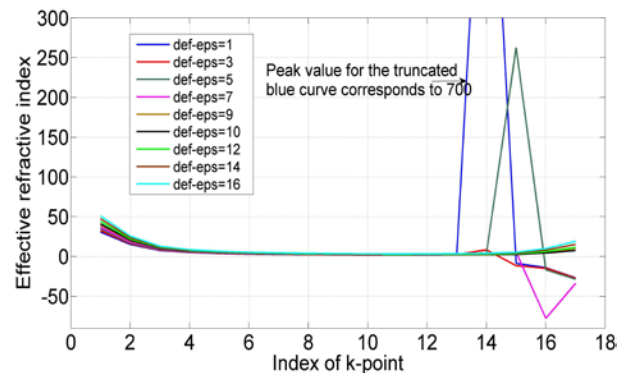
In case of triangular lattice effective index decreases very sharply initially with k-point for almost all defect dielectric constant and then shows a very flat variation with k-points between 4 and 14. Further they rise very sharply at the extreme k-points 15 to 17. In the flatter region of variation the effective index increases with increase in defect dielectric constant as shown in Fig. 15.



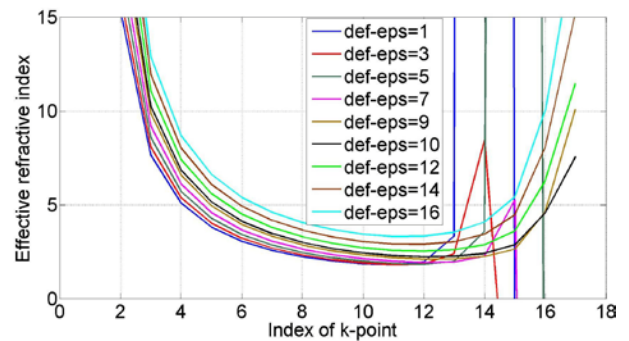
**Figure 15.** Variation of effective refractive index of triangular lattice structure against index of k-point for different defect dielectric constants

Just like the triangular case the similar variation pattern is observed in case of square lattice also as shown in

Fig. 16. On the steep rise at higher k-point anomalous behaviour is observed for defect dielectric constant values from 1 to 8 due to their anomalous pattern in waveguide mode characteristics as shown in Fig. 5. Here also, in the flatter region effective index increases with increase in dielectric constant.



**Figure 16a.** Variation of effective refractive index of square lattice structure against index of k-point for different defect dielectric constants

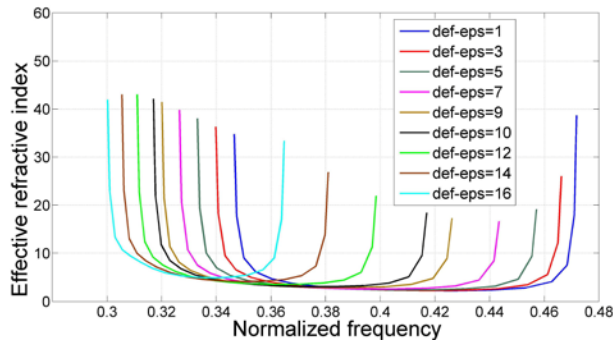


**Figure 16b.** Variation of effective refractive index of square lattice structure against index of k-point for different defect dielectric constants resolved in the Y-axis range of 0 to 15

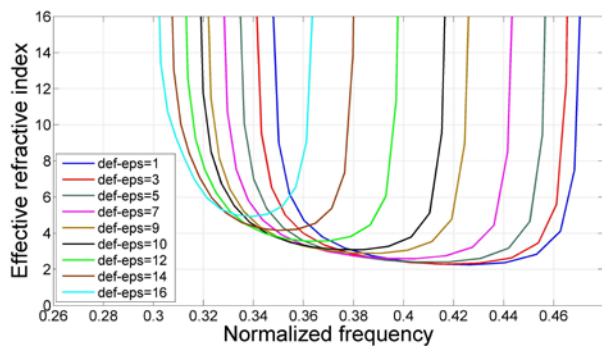
**Variation of Effective refractive index with frequency:**

In case of triangular lattice, for extreme values of frequencies (lower and upper ends) of any waveguide mode the effective refractive index is high and its variation is steep. In between these regions (either ends) the values of effective index is low and the variation is relatively flat. The above two observations are in confirmation to the group velocity variations as shown in Fig. 17a. Effective refractive index can never be negative for triangular lattice structure. A resolved plot (Fig. 17b) shows the refractive index variation in the flatter region. This variation is very small for any

curve with frequency values and also relative to themselves.



**Figure 17a. Variation of effective refractive index of triangular lattice structure against normalized frequency for different defect dielectric constants**

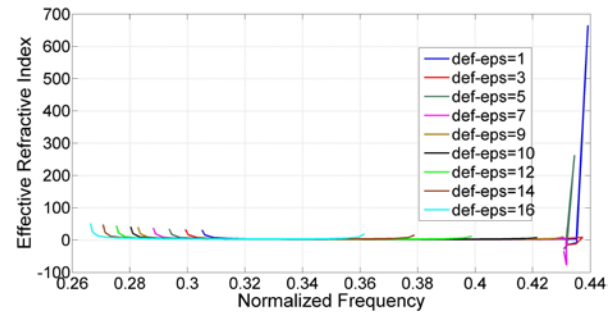


**Figure 17b. Variation of effective refractive index of triangular lattice structure against normalized frequency for different defect dielectric constants resolved in Y-axis 0 to 12**

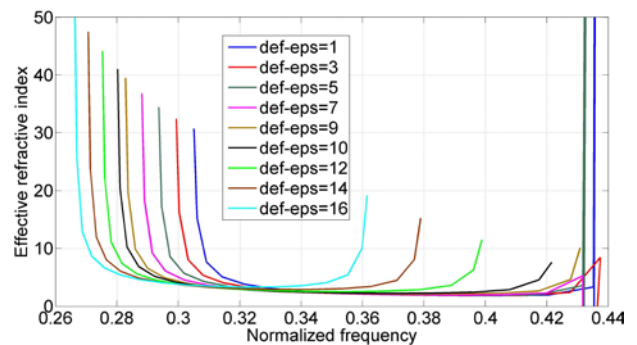
In the case of square lattice structures, with increase in frequency for all defect dielectric constant cases effective index undergoes very steep decrease and then shows flat variation with low values as shown in Fig. 18a. We find anomalous behaviour at the right extreme of frequency axis for defect dielectric constants 1 to 8, where as for higher defect dielectric constants i.e. 9 to 16 the behaviour of the curve is normal and is similar to that of triangular lattice structure. Because of this anomalous behaviour effective refractive index shoots up to a very high value for defect dielectric constants 1 to 8 and then plunges below zero to a small negative value in the right extreme region (Fig. 18b).

A resolved plot (Fig. 18c) shows the refractive index variation in the flatter region. This variation is very

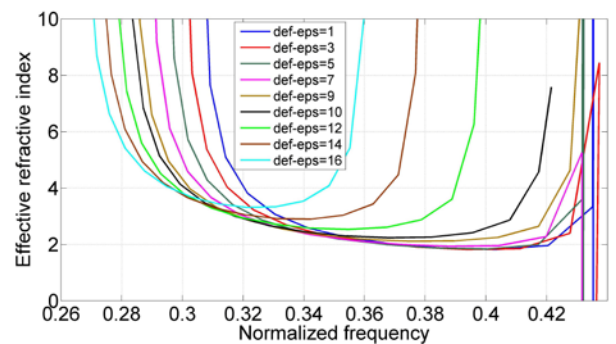
small for any curve with frequency values and also relative to themselves.



**Figure 18a Variation of effective refractive index of square lattice structure against normalized frequency for different defect dielectric constants**



**Figure 18b. Variation of effective refractive index of square lattice structure against normalized frequency for different defect dielectric constants resolved in Y-axis range 0 to 50**

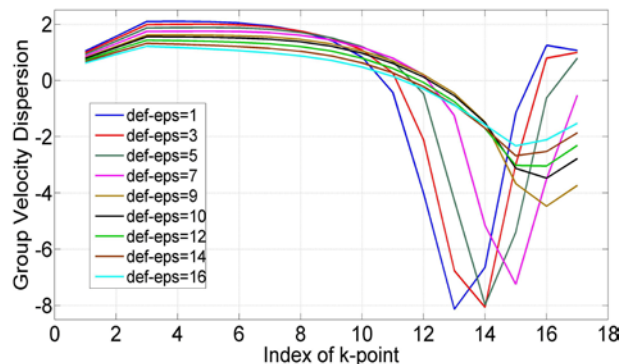


**Figure 18c. Variation of effective refractive index of square lattice structure against normalized frequency for different defect dielectric constants resolved in Y-axis range 0 to 10**



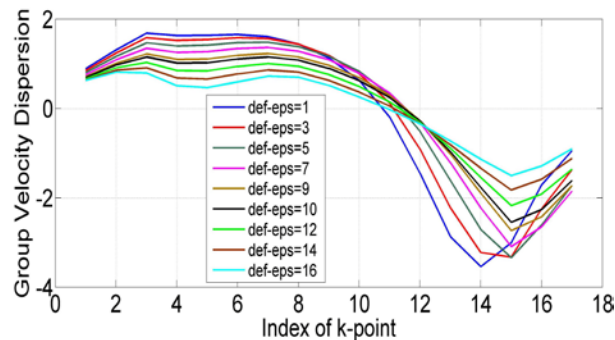
**Variation of GVD with k--point:**

In case of square lattice structure group velocity dispersion slightly increases up to k-point 3 and there onwards it remains almost flatter as shown in Fig. 19, up to k-point 9. Thereafter it starts decreasing gradually for modes corresponding to defect dielectric constants 9 to 16. It falls steeply to a minimum value and subsequently rises steeply for modes corresponding to defect dielectric constants 1 to 8.



**Figure 19. Variation of Group velocity dispersion of square lattice structure against index of k-point for different defect dielectric constants**

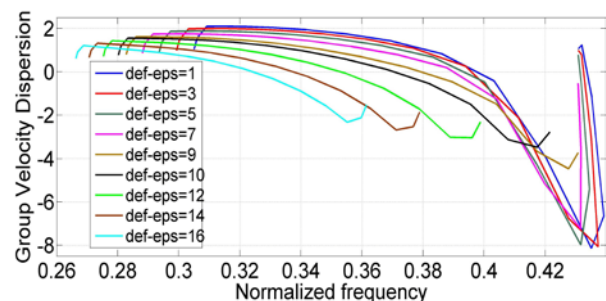
In triangular lattice structure almost similar behaviour is observed, but GVD variation is not as flat as in the case of square lattice structure between k-points 3 and 9 and thereafter it decreases smoothly for all line defect modes. Unlike in the case of square lattice structure the behaviour of curves is uniform as shown in Fig. 20.



**Figure 20. Variation of Group velocity dispersion of triangular lattice structure against index of k-point for different defect dielectric constants**

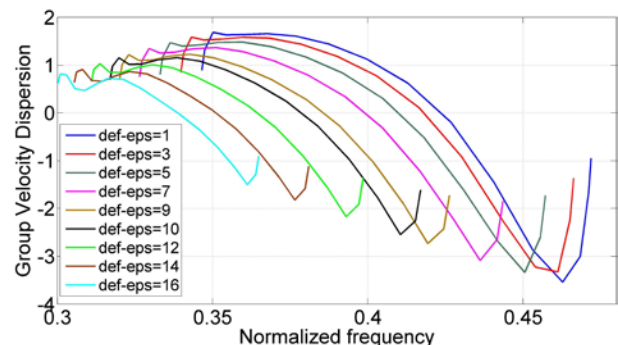
**Variation of GVD with Frequency:**

For square lattice structure GVD increases initially (at lower end of frequency values) with frequency, later it shows flat nature up to few intervals of frequency thereafter it starts decreasing at higher frequencies as shown in Fig. 21. This decrease is gradual for the defect dielectric constant of 9 to 16 and steeper for the defect dielectric constant of 1 to 8 followed by a steep shoot-up at the upper end of frequency values.



**Figure 21. Variation of Group velocity dispersion of square lattice structure against normalized frequency for different defect dielectric constants**

In case of triangular lattice structure GVD shows similar nature, but there is some irregularity initially and there onwards it remains decreases monotonically over some range of frequencies and then it starts rising at the upper end of frequency values as shown in Fig. 22. The range of frequencies of flatter response is not uniform in both square lattices as well as in triangular lattice.



**Figure 22. Variation of Group velocity dispersion of triangular lattice structure against normalized frequency for different defect dielectric constants**

## 6. References

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