Structural Effects on the Photonic Band Structure of Two Dimensional Photonic Crystal

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Abstract

The Photonic band structure of two dimensional Photonic Crystal is calculated using Plane Wave Expansion Method. The structure of the photonic crystal has been varied by changing the radii of the dielectric rods. Three cases have been taken corresponding to different structural forms of silicon, namely c-Si, poly-Si and a-Si materials. The variation of bandgap-to-midgap ratio has been calculated for the fill factor and dielectric contrast. The bandgap to midgap ratio is found to be maximum for a-Si/air structures and shifted to lower values for poly-Si/air and Si/air structures. The results have been explained using the defect migration occurring due to phase transformation from amorphous to crystalline state.

Keywords: 2D Photonic Crystals, Photonic Bandstructure, Plane wave expansion method etc.

Introduction

Photonic crystals have attracted a lot of interest these days due to their tremendous control over light [1, 2]. Photonic crystals are periodic dielectric structures which can exhibit a photonic bandgap (PBG) where light possessing certain values of wave vector is not allowed to propagate in the material. Two-dimensional (2-D) PCs, such as those composed of either dielectric rods or air columns, are widely employed in many applications such as light wave guiding which offer a very high degree of control over light propagation [3]. These are having wide range of applications in optical switches, microscopic lasers, optoelectronic integrated circuits, and optical fibers with photonic crystal cores [4].

In the present paper, the changes of the band structure in 2D photonic crystal have been discussed with the variation in the geometry and the dielectric contrast (disorder)
of the Si material. The width of bandgap is influenced not only by the lattice parameters but also by the dielectric contrast and the fill factor of the photonic crystal’s material. This provides a better understanding of fundamental optical processes in 2D compared to 1D photonic crystal [5, 6].

**Method**

For theoretical method, we have taken a 2D Photonic crystal of square lattice composed of a set of dielectric rods in air. The radius of rod is $r$ and the lattice constant is $a$, with periodicity in x-y plane. The present work has been focused on the wave propagation along the x–y plane with the z component of the wave vector $k_z = 0$.

In TM-polarization mode, the electric field is expanded as a periodic function with period $a$ in the x-direction, prescribed propagation constant $k_x$ with period $a$ in the y-direction and prescribed propagation constant $k_y$. This is given by [7]

$$E(x, y) = \hat{z}E_p(x, y)e^{-ik_x x}e^{-ik_y y}$$

(1)

The wave equation for 2D Photonic crystal is

$$-\frac{\partial^2}{\partial x^2}E(x, y) - \frac{\partial^2}{\partial y^2}E(x, y) = k^2 \varepsilon_r(x, y)E(x, y)$$

(2)

The Fourier series expansion of periodic part of electric field and periodic dielectric constant are

$$E_p(x, y) = \sum_n \sum_q E_{nq}e^{-\frac{2\pi n x}{a}}e^{-\frac{2\pi q y}{a}}$$

and

$$\varepsilon_r(x, y) = \sum_m \sum_p \varepsilon_{np}e^{-\frac{2\pi m x}{a}}e^{-\frac{2\pi p y}{a}}$$

Substituting these values in wave equation (2) and carrying out the algebraic operations, the eigenvalue equation takes the form

$$E_{nq}\left[\left(\frac{2\pi n}{a} + k_x\right)^2 + \left(\frac{2\pi q}{a} + k_y\right)^2\right] = \frac{\omega^2}{c^2}\sum_m \sum_p \varepsilon_{n-m,q-p}E_{mp}$$

(3)

The Fourier coefficient is given as
\[
\varepsilon_{n-m,q-p} = \frac{\pi b^2}{a^2} (\varepsilon_r - 1) \left[ \sqrt{\left(\frac{2\pi(n-m)r}{a}\right)^2 + \left(\frac{2\pi(q-p)r}{a}\right)^2} + \delta_{n-m,q-p} \right]
\]

where \(J_1\) is a Bessel function of first order.

The photonic band structure can be evaluated with above equation (3) for square lattice of Si rods of different structural arrangements in air which shows a band gap in TM polarization case [8].

**Results and Discussion**

**Bandstructure Calculations for Si rods in air**

The photonic band structure is plotted in Fig. 1 for square lattice of crystalline Si rods in air with \(r=0.2a\), which shows a band gap in TM polarization case. The square lattice array has a square Brillouin zone (as shown in Fig.1). The irreducible Brillouin zone is the triangular wedge in the upper right corner; the rest of the Brillouin zone can be related to this wedge by rotational symmetry. The first band has most of its power in the dielectric regions and has a low frequency; the second band has most of its power in the air region and has a higher frequency. An appropriate measure of the degree of concentration of the displacement field in high-\(\varepsilon\) regions is the ratio of the radius of the rods and the lattice spacing defined as the fill factor.

![Figure 1: The photonic band structure for square lattice of Si rod in air with \(r=0.2a\).](image)

**Effect of Fill Factor**

A useful characterization of the photonic band, which is independent of the scale of the crystal, is gap to midgap ratio. Let \(\omega_g\) be the frequency at the middle frequency of the gap and \(\Delta\omega\) be the bandgap frequency, we define the gap to midgap ratio as \(\Delta\omega/\omega_g\). The gap to midgap ratio \((\Delta\omega/\omega_g)\) as a function of fill factor \(r/a\) is plotted in...
Fig. 2 for Si, Poly-Si and Amorphous-Si (a-Si). The radius $r$ of the cylindrical rods is varied to change the fill factor, while the lattice constant $a$ is kept unchanged. For Si, Poly-Si and a-Si, the value of dielectric constants are taken as $\varepsilon = 11.8$, $\varepsilon = 13.8$ and $\varepsilon = 16.36$ respectively.

It is observed that the width of the photonic bandgap first increases with increasing fill factor and then decreases. It is approximately 0.19, 0.18 and 0.17 for Si, Poly-Si and a-Si, respectively. Further, for fill factor greater than a threshold value, the bandgap appears. The threshold fill factor is 0.073, 0.065 and 0.058 for Si, Poly-Si and a-Si, respectively. The range of bandgap in term of fill factor $r/a$ increases with dielectric constant. It is approximately 0.352, 0.363 and 0.372 for Si, Poly-Si and a-Si, respectively.

As fill factor starts to increase from zero, the effective cross-section does not have a significant value. Therefore, the bandgap doesn’t open up. At the resonant condition, the band gap gets maximum value and on both sides it decreases with fill factor ($r/a$). A material with high gap-to-midgap ratio can be used in wide bandgap applications and can be used in filters, reflecters and waveguide for a large bandgap of frequencies. On the other hand, lower value finds applications in localization of the light modes in low frequency bandgap region [3]. Such modes are quantized. In such case, the bound state associated with each number of this family have a different frequency. As the fill factor is increased, the frequency decreases and the field is concentrated more and more in a high $\varepsilon$-region. States with frequency in the center of gap will be most strongly attached to such an arrangement[2].

**Effect of Dielectric Contrast**

From Fig. 3, it is observed that the gap to midgap ratio continuously increasing with dielectric constant for Si rods. It is an established fact that four-fold coordination is preserved even as the Si is transformed from a crystalline state to an amorphous state [9]. The transformation in the amorphous state is primarily related to the long range order which disappear while it transforms to medium range order in polycrystalline
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Si. The bond angles are twisted and this results in the structural disorder when moving from crystalline to amorphous forms [10]. Thus the dielectric constant is increased from c-Si to a-Si and hence a larger dielectric contrast with respect to air background. The bandgap is subsequently increased [2]. The value of photonic band gap/midgap ratio doesn’t get saturated at any value of dielectric contrast, but the slope of the above curve decreases with increase in dielectric contrast. So, there is large change in relative gap with dielectric contrast and as value increases, the change in relative gap is also less. Such a behavior is well known and has been observed by other workers [6, 8].

![Figure 3: Gap to Mid gap ratio with dielectric contrast for fill factor (r/a) = 0.2.](image)

Conclusions
The bandstructure of 2D photonic crystal for Square lattice of Si rods in air has been calculated using Plane wave expansion method. The structural dependence of the bandstructure has been demonstrated for above structures as follows
- The threshold value of fill factor increases from a-Si to c-Si.
- The peak values of gap-to-midgap ratio increases from c-Si to a-Si.
- The gap-to-midgap ratio terminates at the almost same value for fill factor.
- In case of phase transformation the gap-to-midgap ratio decreases as the structure changes from a-Si to c-Si.

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References


