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## Inhibited Spontaneous Emission by Photonic Band Gaps in a Square Lattice of Periodic Dielectric Medium

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INHIBITED SPONTANEOUS EMISSION BY PHOTONIC  
BAND GAPS IN A SQUARE LATTICE OF  
PERIODIC DIELECTRIC MEDIUM

by

Abdullah Al-Ghamdi

A Thesis  
Submitted to the  
Faculty of The Graduate College  
in partial fulfillment of the  
requirements for the  
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Department of Physics

Western Michigan University  
Kalamazoo, Michigan  
August 1991

INHIBITED SPONTANEOUS EMISSION BY PHOTONIC  
BAND GAPS IN A SQUARE LATTICE OF  
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Abdullah Al-Ghamdi, M.A.

Western Michigan University, 1991

The concepts of band theory for electrons can be employed to describe the behavior of electromagnetic waves propagating in two-dimensional, periodic dielectric structures. These two-dimensional, periodic structures can produce photonic band gaps in which the spontaneous emission by atoms embedded in the structure is prohibited and as a result the performance of many semiconductor devices can be enhanced. The calculations are based on finding the eigenvalues of the algebraic equation for the frequencies of electromagnetic waves moving in a square lattice composed of square dielectric rods with different dielectric constants.

## ACKNOWLEDGEMENTS

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Abdullah Al-Ghamdi

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## TABLE OF CONTENTS

ACKNOWLEDGEMENTS .....	ii
LIST OF FIGURES .....	iv
CHAPTER	
I. INTRODUCTION .....	1
II. PHOTONIC BANDS IN PERIODIC MEDIA .....	10
III. CONCLUSION .....	23
REFERENCES .....	26
BIBLIOGRAPHY .....	27

## LIST OF FIGURES

1. First Brillouin Zone With an Illustration of the Symmetric Directions.....	19
2. Plot of Frequency $\omega$ Versus Wave Vector $k$ for Square Lattice of Periodic Dielectric Medium When $\epsilon_A/\epsilon_B = 1$ .....	20
3. Plot of Frequency $\omega$ Versus Wave Vector $k$ for Square Lattice of Periodic Dielectric Medium When $\epsilon_A/\epsilon_B = 5$ .....	21
4. Plot of Frequency $\omega$ Versus Wave Vector $k$ for a Square Lattice of Periodic Dielectric Medium When $\epsilon_A/\epsilon_B = 14$ .....	22

## CHAPTER I

### INTRODUCTION

Spontaneous emission between two excited states of an atom occurs as a result of interactions between the atom and space even in the absence of an external emission field. The emitted light from the spontaneous radiation is not perfectly monochromatic, but instead has a frequency spectrum whose width is inversely proportional to the atomic lifetime  $\tau$ .<sup>1</sup> This width arises from the fact that the longest time during which energy measurements can be made is approximately the atomic lifetime  $\tau$ , and hence the energy difference of the levels is uncertain by the amount

$$\Delta E = \frac{\hbar}{\tau} \quad (1.1)$$

In equation (1.1)  $\hbar$  is Planck constant divided by  $2\pi$ .

The correct description of spontaneous emission processes in accordance with quantum theory was first given by Einstein.<sup>2</sup> Consider, for example, a transition from a state of energy  $E_m$  to a lower energy state  $E_n$ , such that the transition is accompanied by the loss of energy in the atomic system. The energy loss in the atomic system appears as energy in the radiation field, and the frequency of the emitted radiation is given by Bohr's frequency

condition:

$$E_m - E_n = h\nu \quad (1.2)$$

where  $h$  is Planck constant. The energy which appears in the radiation field is in the form of a photon.

To compute the rate of spontaneous emission of electromagnetic radiation Einstein<sup>2</sup> assumes that the probability of a transition of a system in state  $E_m$  to a state of lower energy level  $E_n$  with the emission of a photon of radiation of frequency given by the Bohr frequency condition is

$$\text{Probability of radiation} = [A + B_{mn}\rho(\nu)] N_m \quad (1.3)$$

Here  $A$  is the probability of spontaneous emission; the term  $B_{mn}\rho(\nu)$  is a probability of induced emission, and  $N_m$  is the number of excited atoms in the higher energy state  $E_m$ . Hence the transition from the higher energy state  $E_m$  to the lower energy state  $E_n$  may take place with the help of electromagnetic radiation or by a spontaneous process. Conversely, for a transition from a lower state  $E_n$  to a higher energy level  $E_m$ , with the absorption of a photon of radiation, the probability of absorption according to Einstein<sup>2</sup> is

$$\text{Probability of absorption} = [B_{nm}\rho(\nu)] N_n \quad (1.4)$$

where  $N_n$  is the number of the atoms occupying the energy level  $E_n$ .

For an atom in free space, when the steady state is reached, the energy balance of emitted to absorbed radiation requires that,

Probability of radiation = Probability of absorption

Thus,

$$[A + B_{mn} \rho(\nu)] N_m = [B_{nm} \rho(\nu)] N_n \quad (1.5)$$

This condition, equation (1.5), predicts a spectral distribution given by

$$\rho(\nu) = \frac{A}{B_{mn}} \frac{1}{\left(\frac{B_{nm}}{B_{mn}}\right) \exp\left(\frac{h\nu}{KT}\right) - 1} \quad (1.6)$$

In equation (1.6), under the condition of thermal equilibrium, the populations of the states are, according to Boltzmann's relation, given by

$$\frac{N_n}{N_m} = \exp \frac{\Delta E}{KT} \quad (1.7)$$

On the other hand, the Planck law of black body radiation is

$$\rho_{(v)} = \frac{8\pi h\nu^3}{c^3} \frac{1}{\exp\left(\frac{h\nu}{KT}\right) - 1} \quad (1.8)$$

A comparison of equation (1.6) with (1.8) yields,

$$B_{mn} = B_{nm} = B$$

and

$$\frac{A}{B} = \frac{8\pi h\nu^3}{c^3} \quad (1.9)$$

In equation (1.9), the ratio of the coefficients for stimulated and spontaneous emission depends only on the frequency of the photon involved.

Spontaneous emission processes are important to us as they play a fundamental role in determining the optical properties of materials. For instance, spontaneous emission dominates many characteristics of an atom through its decreasing of the lifetime of atomic excited states. The performance of many semiconductor devices such as semiconductor lasers, heterojunction bipolar transistors, and solar cells, are all limited due to the loss of energy caused by spontaneous emission. Consequently, many researchers have been involved in studying methods which can be used to inhibit the spontaneous emission by atoms in solid state systems and devices.

In fact, it has been recognized for a long time that spontaneous emission is not necessarily a fixed and

immutable property of the coupling between matter and space, but it can be controlled by modification of the properties of the radiation fields which form the environment of a single radiating atom of the system. The starting point of these observations was made many years ago by Purcell,<sup>3</sup> when he found that the spontaneous emission rate for a two-state atomic system is increased if the atom is surrounded by a cavity tuned to the transition frequency,  $\nu$ . If, on the contrary, the cavity is mistuned and  $\nu$  lies below the fundamental frequency of the cavity, spontaneous emission is inhibited.

Additional evidence of inhibition of spontaneous emission has been found experimentally by a number of workers on electron and single atom systems. One of the first observations of inhibition of the spontaneous emission in electron systems was made by Gabrielse and Dehmelt.<sup>4</sup> They presented evidence where they found that the radiative decay of the cyclotron motion of a single electron is significantly inhibited when the electron is in thermal equilibrium at nearly 4K and is located within a microwave cavity formed by the electrodes of a penning trap. The penning trap is used to confine the electron in a region of space which has a certain natural cavity oscillation frequency. They observed damping times as much as 5 times longer than the free space value and attributed

the increased lifetime to cavity resonance effects from the surrounding electrodes. Basically, this experiment provided convincing evidence that spontaneous emission can be suppressed by employing structures which have natural oscillation frequencies. Subsequently, Hulet, Hilfer and Kleppner<sup>5</sup> observed that the spontaneous emission of radiation is inhibited in atoms of certain Rydberg states which are placed in a resonance cavity rather than free space. They used a cavity consisting of two plates that are separated by six disk-shaped quarter spacers to eliminate the vacuum modes at the transition frequency. When the wavelength ( $\lambda$ ) is less than  $2d$ , where  $d$  is the distance between the plates, the atomic emission rate is enhanced relative to its free-space value. As the separating distance was reduced, and the radiation wavelength ( $\lambda$ ) became greater than  $(2d)$ , they observed the spontaneous emission to "turn off" abruptly at the cutoff frequency of the waveguide-like structure and the natural lifetime of the atom was measured to increase in this process by a factor of at least 20.

These studies are evidence of how significant effort has been put into developing methods to inhibit the spontaneous emission by atoms. The common goal of these studies is to find a means of opening a photonic band gap or forbidden region in the electromagnetic frequency



spectrum, so as to prohibit the propagation of the electromagnetic waves away from a spontaneously emitting atom which is placed in the structure. One illustration of the usefulness of photonic band gaps occurs in the design of laser mirrors. If an optical wave falls in the forbidden band gap of a mirror constructed of layered quarterly plates, such a wave will be evanescent in the mirror and will not be able to propagate in the medium. Thus, these light waves will be reflected from the quarter wave plate array which form a highly reflecting mirror.

One way of developing an optical structure with band gaps, which has been of considerable interest in recent years, is to create a dielectric medium with a periodic dielectric structure. Such periodic structures are well known, from the theory of electron and phonons in crystals, to exhibit band gaps and the theory of these gaps has been well understood for over 50 years. In periodic dielectrics, as in electron and phonon systems, a band structure is introduced in the periodic optical medium along with the associated concepts of an optical reciprocal lattice, Bloch wave functions, etc. The mathematics of periodic structure can be applied to electromagnetic waves with little change from its original application to the study to electronic waves and phonons. We shall be concerned with these types of periodic

dielectric structures in this thesis.

The first studies of photonic bands periodic lattices were made by Yabonovitch,<sup>6</sup> who based his work on a three-dimensional faced-centered-cubic (Fcc) periodic structure. His studies addressed experimentally the possibility of inhibited spontaneous emission with possible application to semiconductor lasers, heterojunction bipolar transistors, and solar cells as follows:

1. In semiconductor lasers, the inhibition of spontaneous emission at frequencies other than the lasing frequency prevent energy losses by these mechanisms.

2. In bipolar junction transistors the current gain can be enhanced if the electron-hole recombination rate is minimized. This can be accomplished by the suppression of certain spontaneous emission mechanisms.

3. In solar cells, the suppression of certain spontaneous emission mechanisms leads to higher efficiency in the conversion of solar energy.

In a recent experiment by Yablonovitch and Gmitter<sup>7</sup> the concepts of band theory are used to describe the behavior of electromagnetic waves in three-dimensional periodic face-centered-cubic dielectric structures. They found experimentally that an open photonic band gap can indeed be achieved in the three-dimensional dielectric structures, but it requires a dielectric index contrast nearly in 3.5

to 1.

The purpose of this thesis is to study the photonic band gap in two-dimensional periodic structure lattice. Our goal is to find an open band gap in these types of periodic dielectric structures. We calculate the band structure using the standard eigenvalue methods which are described in the next section. The computation of photonic band structures has become of great theoretical interest in the last three years.

## CHAPTER II

### PHOTONIC BANDS IN PERIODIC MEDIA

Electrons in periodic structures are arranged in energy bands separated by regions (gaps) in energy for which no wave-like electron orbitals exist. Such forbidden regions are called band gaps and the origins of these energy gaps are in the Bragg reflection of electron waves in crystals from the periodic positive ion background. The theory of band gaps for electrons and phonon is well known. Applications of the well-known mechanisms for gap formation in electron and phonon systems to photonic systems are now possible and have recently been of interest for one-dimensional, two-dimensional, and three-dimensional periodic dielectric structures. This means that the concepts of reciprocal lattice, Bloch wave functions, etc., may now be applicable to photonic waves in periodic dielectric media.

The wave function which describes the motion of electron waves in a one-dimensional lattice is given by the time-independent Schrodinger's equation

$$\left[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right] \psi = E\psi \quad (2.1)$$

where  $V$  is a periodic potential and  $E$  is the energy eigenvalue.

In the wave equation (2.1) the potential  $V(x)$  is periodic in  $x$  with

$$V(x) = V(x+a) \quad (2.2)$$

where  $a$  is the lattice constant. This means that an observer at  $x$  sees essentially the same potential as an observer at  $x + a$ . The solution of the Schrodinger's equation for the periodic potential  $V(x)$  was proved by F. Bloch to be of the form,

$$\psi_k(x) = U_k(x) \exp(ikx) \quad (2.3)$$

where

$$U_k(x) = U_k(x+a) \quad (2.3a)$$

is periodic in the lattice. Here the subscript  $k$  on  $U$  indicates that  $U$  depends on  $k$  where  $k$  is the Bloch wave vector.

If we consider the potential energy  $V(x)$  in a linear lattice with lattice constant  $a$ , the potential may be expanded in a Fourier series as,

$$V(x) = \sum_G V_G e^{iGx} \quad (2.4)$$

where  $G$  is reciprocal lattice vector. The wave function in (2.3) can also be expressed as a Fourier series summed over all value of wave vectors as

$$\psi(\mathbf{x}) = \sum_{\mathbf{k}} C(\mathbf{k}) e^{i\mathbf{k}\mathbf{x}} \quad (2.5)$$

where  $C(\mathbf{k})$  are the Fourier coefficients.

Using equation (2.4) and (2.5) in (2.1) the wave equation can be rewritten as an algebraic equation

$$\sum_{\mathbf{k}} \frac{\hbar^2}{2m} k^2 C(\mathbf{k}) e^{i\mathbf{k}\mathbf{x}} + \sum_{\mathbf{g}} \sum_{\mathbf{k}} V_{\mathbf{g}} C(\mathbf{k}) e^{i(\mathbf{k}+\mathbf{g})\mathbf{x}} - \epsilon \sum_{\mathbf{k}} C(\mathbf{k}) e^{i\mathbf{k}\mathbf{x}}, \quad (2.6)$$

and equation (2.6) can be rearranged as

$$\left( \frac{\hbar^2}{2m} k^2 - \epsilon \right) C(\mathbf{k}) + \sum_{\mathbf{g}} V_{\mathbf{g}} C(\mathbf{k}-\mathbf{g}) = 0. \quad (2.7)$$

The solution of equation (2.7) for the wave function is then

$$\psi_{\mathbf{k}}(\mathbf{x}) = \sum_{\mathbf{g}} C(\mathbf{k}-\mathbf{g}) e^{i(\mathbf{k}-\mathbf{g})\mathbf{x}} \quad (2.8)$$

which may be rewritten as

$$\psi_{\mathbf{k}}(\mathbf{x}) = \left( \sum_{\mathbf{g}} C(\mathbf{k}-\mathbf{g}) e^{-i\mathbf{g}\mathbf{x}} \right) e^{i\mathbf{k}\mathbf{x}} = U_{\mathbf{k}}(\mathbf{x}) e^{i\mathbf{k}\mathbf{x}} \quad (2.9)$$

If we define  $U_{\mathbf{k}}(\mathbf{x})$  as

$$U_{\mathbf{k}}(\mathbf{x}) = \sum_{\mathbf{g}} C(\mathbf{k}-\mathbf{g}) e^{i\mathbf{g}\mathbf{x}} \quad (2.9a)$$

then  $U_{\mathbf{k}}(\mathbf{x})$  is a Fourier series over the reciprocal lattice vectors, and as a result it is invariant under crystal lattice translation  $\mathbf{T}$ . So,

$$U_{\mathbf{k}}(\mathbf{x}) = U_{\mathbf{k}}(\mathbf{x} + \mathbf{T}) \quad (2.10)$$

The matrix for equation (2.7) can also be solved for the electron dispersion relation in  $\epsilon(\mathbf{k})$ . There we find, for a one-dimensional periodic structure like that of equation (2.7), a band gap in the electron dispersion relation occurs at  $\mathbf{k} = \pm \pi/a$  (edges of the first Bravais zone).

The vector ( $\mathbf{G}$ ) is known as a reciprocal lattice vector and in a one-dimensional periodic medium ( $\mathbf{G}$ ) is parallel to X-axis. The reciprocal lattice vector and direct lattice vector which describe the atomic positions belong to the same lattice system and the gaps in the electron dispersion relation open up for  $\mathbf{k}$  when

$$\mathbf{k} = (2n+1)\mathbf{G}/2 \quad (2.11)$$

where  $n=0, \pm 1, \dots$ . The gaps in the dispersion relation are then a manifestation of the Bragg scattering of the electron waves by the crystal lattice.

In a three-dimensional system the reciprocal lattice vector  $\mathbf{G}$  has three vector components as,

$$\mathbf{G} = h \mathbf{A} + k \mathbf{B} + l \mathbf{C} \quad (2.12)$$

Where  $h$ ,  $k$ , and  $l$  are integers and called Miller indices. The fundamental vectors  $\mathbf{A}$ ,  $\mathbf{B}$ , and  $\mathbf{C}$ , which have units of reciprocal distance, are not necessarily orthogonal and

none of them are necessarily parallel to any direct lattice vector. The three vector components of the reciprocal lattice are defined by

$$A = 2\pi \frac{b \times c}{a \cdot (b \times c)} \quad (2.13)$$

$$B = 2\pi \frac{c \times a}{a \cdot (b \times c)} \quad (2.14)$$

$$C = 2\pi \frac{a \times b}{a \cdot (b \times c)} \quad (2.15)$$

where  $a$ ,  $b$ , and  $c$  are the direct lattice vectors. Moreover, we can find the volume of reciprocal lattice for a unit cell as

$$\Omega = |A \cdot (B \times C)| \quad (2.16)$$

When equation (2.11), (2.14), and (2.15) are used to substitute for  $A$ ,  $B$ , and  $C$  respectively the result is

$$\Omega = \frac{8\pi^3}{\tau} \quad (2.17)$$

where  $\Omega$  is the volume of the direct lattice.

In a three-dimensional periodic dielectric structure a similar calculation to that given above shows that a band gap also exists. Again gaps in the dispersion relation open up for

$$2\mathbf{k} \cdot \mathbf{G} + G^2 = 0 \quad (2.18)$$

for  $\mathbf{G}$  a translation vector of the three dimensional



reciprocal lattice vector.<sup>8</sup> Waves with frequencies in the forbidden bands of the dispersion relation, as in one dimension, do not propagate, but are evanescent due to Bragg reflection.

The light wave traveling in a two-dimensional periodic structure should be described similarly to the quantum theory of electrons in crystals, and thus, the concept of Bloch modes, forbidden gaps, and evanescent wave will apply. However, there are some contrasts between electronic and photonic band structures which are as follows:

1. The basic dispersion relation for electrons is parabolic, while that for photons is linear;
2. The spin for electrons is  $\pm 1/2$ , while that for photons is  $\pm 1$ ;
3. The band theory of electrons is only an approximation, while the photonic band theory is exact, due to the fact that, if the photon-photon interaction is negligible.

The calculation we make for photonic band gaps in a two-dimensional periodic structure is based on the application of the band theory of periodic structures to study the propagation of electromagnetic waves in a square lattice arrangement of dielectric rods of differing dielectric constant. The two contrasting reflective

indices in the square lattice arrangement of dielectric rods will control the behavior of the band gap in the dispersion relation of the light. We assume that square rods of dielectric material with dielectric constants  $\epsilon_A$  and  $\epsilon_B = 1$ , are embedded in a two dimensional square lattice periodic structure. The rods have sides of length equal to  $a_0 / \sqrt{2}$ , where  $a_0$  is the lattice constant, and hence form a checkerboard pattern.

To obtain the dispersion relation for propagation in the period structure we need to solve Maxwell's equations

$$\nabla \times \vec{B} = i \frac{\omega}{c} \epsilon(\vec{X}) \vec{E} \quad (2.19)$$

$$\nabla \times \vec{E} = -i \frac{\omega}{c} \vec{B} \quad (2.20)$$

where  $\epsilon(\vec{X}) = \epsilon(x, y)$  is the periodic dielectric constant for the electromagnetic modes of the structure. Expanding these Maxwell equations in a Fourier series taking  $\vec{E} = (0, 0, E)$

$$\vec{E} = \sum_{\vec{G}} A(\vec{K}|\vec{G}) e^{i(\vec{K}+\vec{G}) \cdot \vec{r}} \quad (2.21)$$

where  $\vec{G}$  are the reciprocal lattice vectors of the square lattice we obtain for light propagating parallel to the X-Y plane, the eigenvalue equation

$$\sum_{\vec{G}'} |\vec{k} + \vec{G}| |\vec{k} + \vec{G}'| \hat{K}(\vec{G} - \vec{G}') A(\vec{k} | \vec{G}') = \frac{\omega^2}{C^2} A(\vec{k} | \vec{G}) \quad (2.22)$$

where

$$\hat{K}(\vec{G} - \vec{G}') = \frac{1}{\epsilon_A \vec{G}_0} \delta + \frac{1}{2} \left( \frac{1}{\epsilon_B} - \frac{1}{\epsilon_A} \right) f(G_1) f(G_2) \quad (2.23)$$

and

$$F(G_\alpha) = 1 \quad G = 0 \quad (2.24)$$

$$= -2 \frac{\sin(G_\alpha, a)}{G_\alpha, a} \quad G \neq 0 \quad (2.24a)$$

with the length of the side of a square dielectric given by (a).

We solve the matrix numerically on computer to find the complex eigenvalue using a 100 x 100 matrix and choosing the lowest three bands to study the photonic band gaps. The rods which are embedded in the square lattice are vacuum and dielectric with dielectric ratio taken as,

$$\epsilon_A / \epsilon_B = 1, 5, 14.$$

The results are presented for  $\omega$  (frequency) versus  $k$  (wave vector) along the three symmetry axes of the first Brillouin zone as follows (see Figure 1): (a) from point 0 to A, (b) from point A to B, and (c) from point B back to 0. An illustration of these directions is shown in Figure 1.

Illustrations of photonic band gaps for different

dielectric constants of the embedded square rods, which are calculated in terms of the eigenvalue of algebraic equation, are shown in Figures 2 to 4.

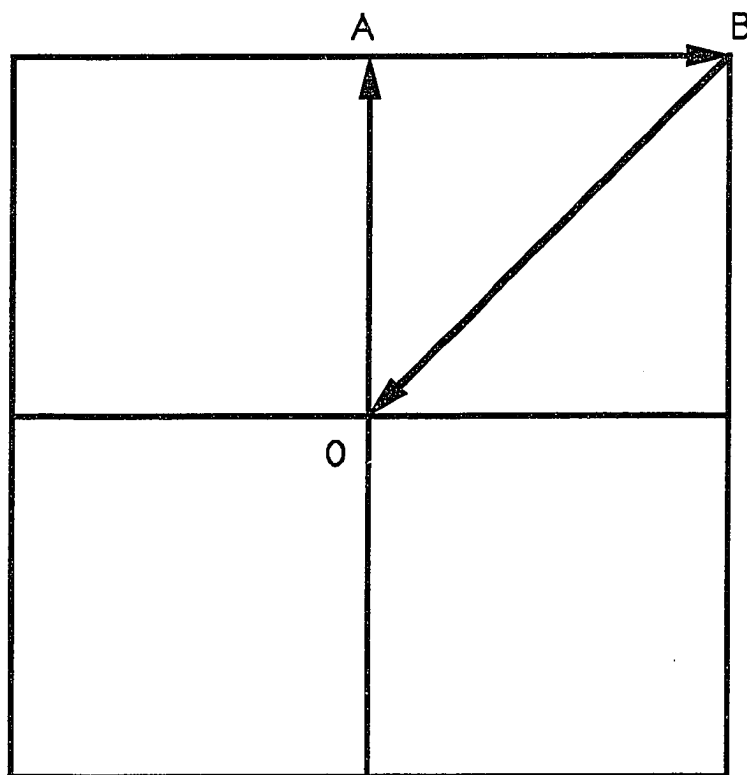


Figure 1. First Brillouin Zone With an Illustration of the Symmetric Directions.

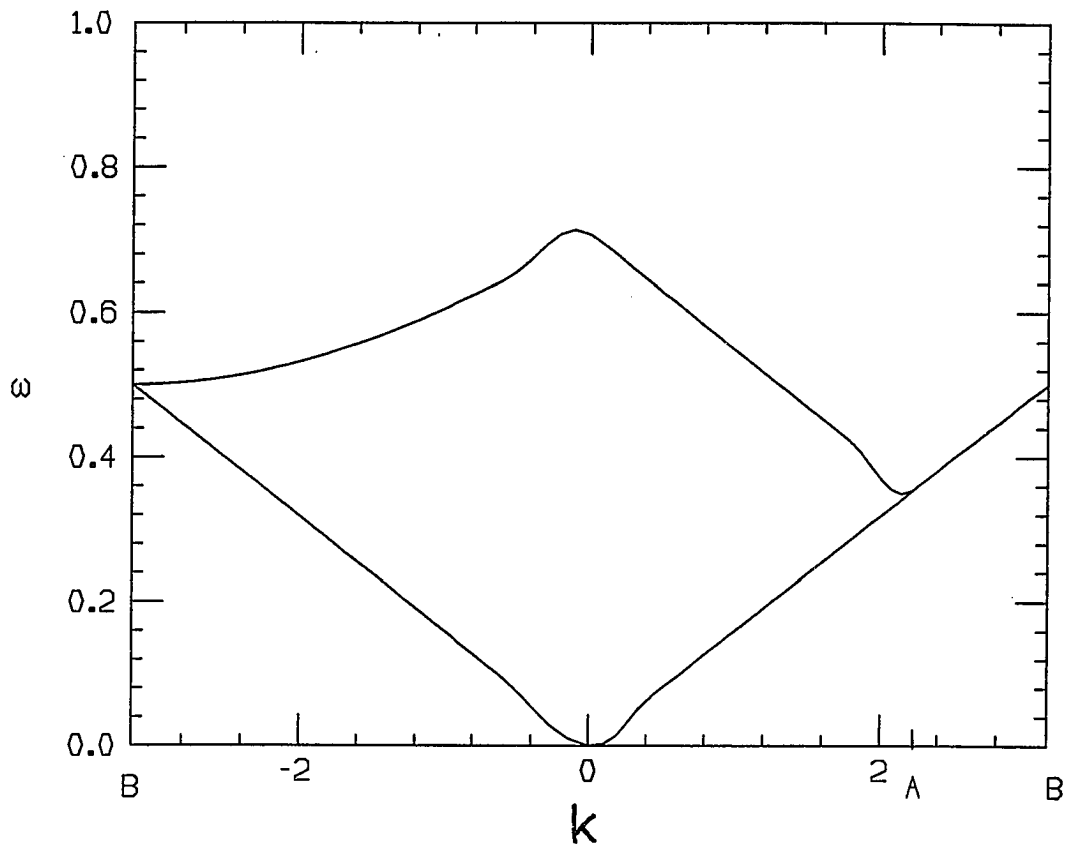


Figure 2. Plot of Frequency  $\omega$  Versus Wave Vector  $k$  for Square Lattice of Periodic Dielectric Medium When  $\epsilon_A/\epsilon_B = 1$ .

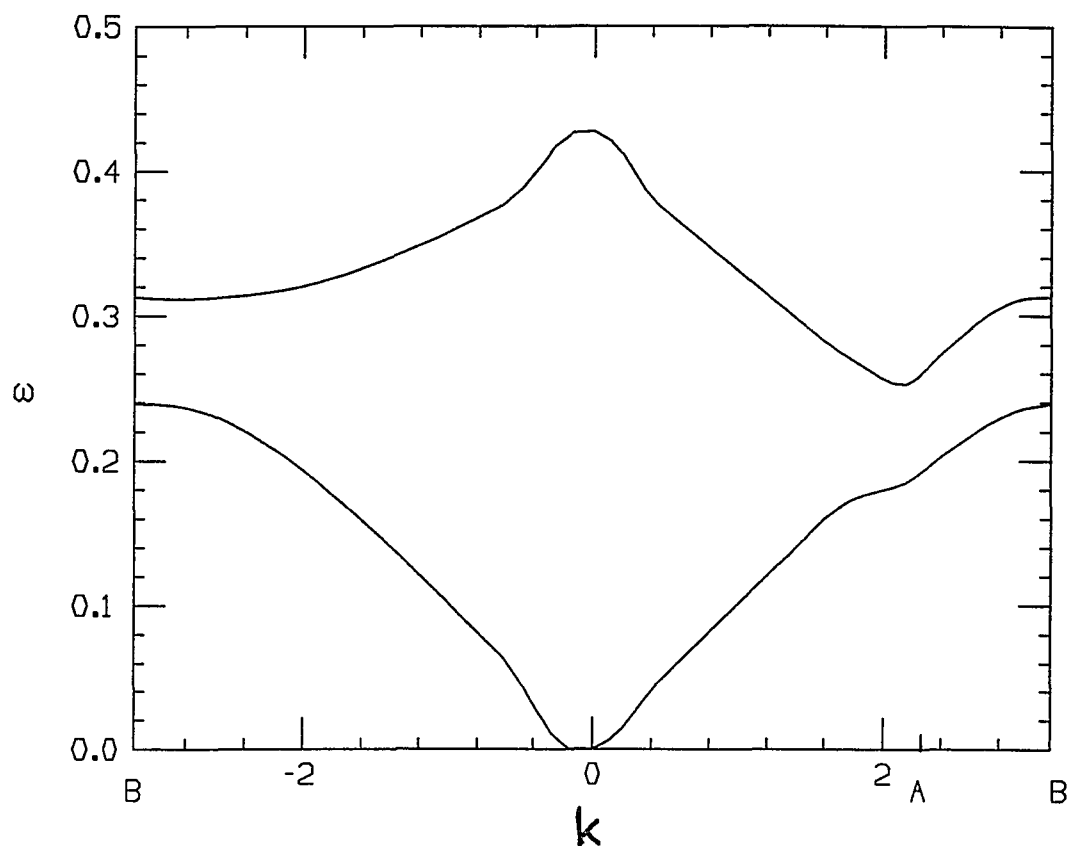


Figure 3. Plot of Frequency  $\omega$  Versus Wave Vector  $k$  for Square Lattice of Periodic Dielectric Medium when  $\epsilon_A/\epsilon_B = 5$ .

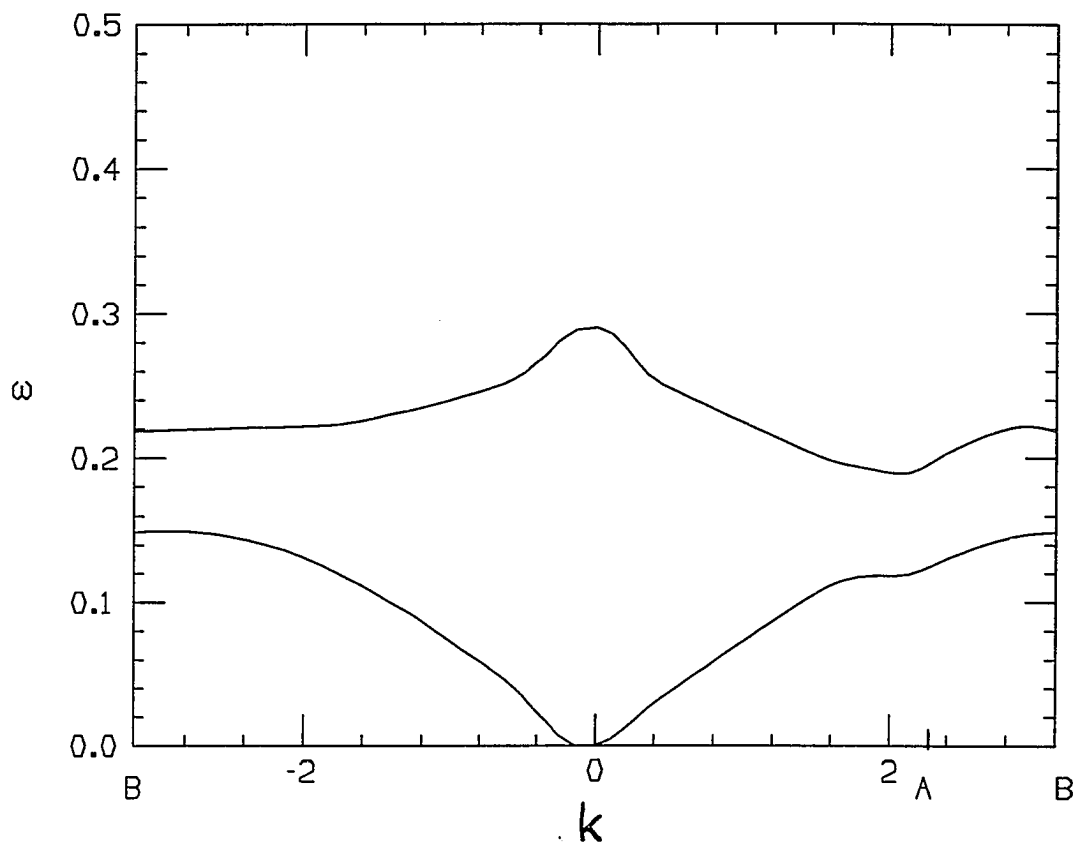


Figure 4. Plot of Frequency  $\omega$  Versus Wave Vector  $k$  for a Square Lattice of Periodic Dielectric Medium When  $\epsilon_A/\epsilon_B = 14$ .



## CHAPTER III

### CONCLUSIONS

The propagation of light in a two-dimensional periodic dielectric medium can best be described in terms of Maxwell's equations written in terms of a periodic permeability tensor  $\epsilon$ . In periodic dielectric media these equations are then

$$\nabla \times \vec{H} = i\omega\epsilon\vec{E} \quad (3.1)$$

$$\nabla \times \vec{E} = -i\omega\mu\vec{H} \quad (3.2)$$

where  $\omega$  is the frequency of the light,  $\vec{E}$  and  $\vec{H}$  are the electric and magnetic fields.

Substituting equation (3.2) in equation (3.1) the electric field can be written as a wave equation

$$\nabla \times (\nabla \times \vec{E}) - \omega^2\epsilon\mu\vec{E} = 0 \quad (3.3)$$

where  $\epsilon$  is periodic function in the lattice.

The dielectric tensor  $\epsilon$ , in the periodic media, can be expanded as a Fourier Series

$$\epsilon(\mathbf{x}) = \sum_{\mathbf{G}} \epsilon_{\mathbf{G}} e^{-i\mathbf{G}\cdot\mathbf{x}} \quad (3.4)$$

where  $\mathbf{G}$  is a reciprocal lattice vector in the two-dimensional lattice.<sup>9</sup> We shall take  $\vec{E}$  to be parallel to

the dielectric rods, then in equation (3.3) standard methods developed by Bloch for the study of the motion of electron waves in a periodic lattice can be used to obtain a solution of equation (3.3) in term of Bloch wave photonic states. We have done this in section II for light propagating in a two-dimensional checkerboard pattern and studied the dispersion relation for photonic propagating modes in this structure. Our study has concentrated in the opening up of photonic gaps, in the periodic structure. In such gaps the electromagnetic radiation is evanescent (non-propagating). This attribute may play a significant role in future development of electronic devices because it will increase the efficiency of many such semiconductor devices. Many semiconductor devices, such as semiconductor lasers, hetrojunction bipolar transistors, and solar cells, are all limited in their performance by energy losses by spontaneous emission. The opening up of photonic band gaps in semiconductor devices by introducing a periodic dielectric constant, will play a decisive role in inhibiting the spontaneous emission in these devices. Therefore by choosing the particular material the performance of many devices will be strongly increased.

In conclusion, the dielectric tensor contrast between the media and the dielectric rod in our checkerboard media allows us to find photonic band gaps in the dispersion

relation of light in term of the energy eigenvalues from Maxwell's equation, which are measured in units of  $(2\pi/a)$ , where  $a$  is the side of the simple cube. In the case of a band gap the electromagnetic wave is evanescent and the propagation of light is prohibited.

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