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Yi-Fen Chang

Western Michigan University

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IMPURITY MODES IN PHOTONIC BAND STRUCTURES

by

Yi-Fen Chang

A Thesis
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Faculty of The Graduate College
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IMPURITY MODES IN PHOTONIC BAND STRUCTURES

Yi-Fen Chang, M.A.
Western Michigan University, 1993

In this thesis I study a theoretical model of one-dimensional dielectric array (a layered system of dielectric slabs) which forms a periodic dielectric system in which band gaps are opened in the frequency spectrum. Specifically, we study such a one-dimensional array with linear impurities introduced in the periodic dielectric system. In these impurity structures narrow resonant modes are found in the band gaps as impurity modes and these impurity modes change with the dielectric constant. This impurity problem is similar to the donor and acceptor state problem in electronic semiconductors. The calculations presented in this thesis are based on numerically studying impurity modes from linear impurities in an otherwise periodic one dimensional array of dielectric slabs and determining the impurity mode frequency as a function of the impurity dielectric constant of the impurity slabs.
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Yi-Fen Chang
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CHAPTER I

INTRODUCTION

In this thesis, I am interested in the propagation of light in a one-dimensional periodic dielectric array. As in systems in which electrons move in the periodic potential formed by the atoms in a crystal, there is in periodic optical system a band structure with band gaps in which no excitations (light) can propagate in the array. These band structures have been named photonic band structures, and light with frequencies in the band gaps is totally absent from the system, just as electrons with energies in the band gaps of materials or semiconductors cannot propagate in these electrical systems. As a result of frequency gaps, for example, spontaneous emission by atoms embedded in periodic optical structures is prohibited if the frequency of spontaneous emission lies within an optical band gap. As we shall see below, this suppression of spontaneous emission enhances the performance of many semiconductor devices. In addition, I will specifically look at the problem of the light propagating in the 1-D periodic array in the presence of an impurity dielectric slab. This impurity problem is similar to the donor and acceptor state problem in electronic semiconductors. I
wish to determine the conditions needed to observe donor and acceptor levels in our 1-D slab system. I will use the computer to do the problem by solving essential exactly, the analytic expressions which I obtain for the description of the propagation of light in our system.

What I am trying to do is to open an energy gap that does to photons what the periodic ion potential in semiconductors does to electrons. As we mentioned above, spontaneous emission processes play a fundamental role in determining the electronic optical properties of many types of materials used in science and technology. For instance, spontaneous emission dominates many characteristics of an atom through its decreasing 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. And this interest has spread to all aspects of the propagation of light in periodic and doped periodic optical systems.

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
radiation fields, specifically, density of states of the radiation fields which form the environment for a single radiating atom of the system. These observations were made many years ago by Purcell. He found that the spontaneous emission rate for a two-state atomic system is increased when the atom is surrounded by a cavity tuned to the transition frequency $v$. This arises from the increase in the electromagnetic modes available to decay into at the cavity resonance frequency. Therefore, when the cavity is mis-tuned and $v$ lies away from the fundamental frequency of the cavity, spontaneous emission is inhibited due to the absence of electromagnetic modes available for the atom to decay into.

Other evidence of inhibition of spontaneous emission has been found by other workers on electron and single atom system. Gabrielse and Dehmelt found that the radiative decay of the cyclotron motion of a single electron is inhibited when the electron is in thermal equilibrium at nearly 4°K and is located within a microwave cavity formed by the electrodes of a Penning trap. 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. Their experiment provided evidence that spontaneous emission can be suppressed by employing structures which have natural oscillation frequencies. Subsequently, Hulet, Hilfer and
Kleppner observed that spontaneous emission is inhibited in atoms of certain Rydberg states which are placed in a resonance cavity rather than free space. They set the cavity by two plates that are separated by six disk-shaped quarter wave spacers to eliminate the vacuum modes at the transition frequency. When the wavelength is less than 2 times the distance between the plates, the atomic emission rate is enhanced relative to its free-space value. When the separating distance was reduced, they observed the spontaneous emission to "turn off" abruptly at 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. The application of photonic band gaps also occurs in the design of laser mirrors. If the optical wave falls in the forbidden band gap of a mirror constructed of layered quarter plates, the wave will be evanescent in the mirror and will not be able to propagate in the medium. Therefore, these light waves will be
reflected from the quarter wave plate array which forms a highly reflecting mirror. These studies illustrate the usefulness of photonic band gaps in practical applications.

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. In periodic dielectrics, as in periodic electron system, a band structure is introduced in the periodic optical medium along with the associated concepts of an optical reciprocal lattice, Bloch wave functions, etc. Yablonovitch worked on a three-dimensional face-centered-cubic periodic optical structure. His studies address experimentally the possibility of inhibited spontaneous emission with possible application to semiconductor lasers, heterojunction bipolar transistors, and solar cells. Yablonvitch and Gmitter used the concepts of band theory 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 of nearly 3.5 to 1.

Most recently, Yablsonvitch created a photonic "crystal" that works in the microwave region. The photonic crystal is a dielectric substance in which holes about 45 millimeters in diameter have been drilled at three dif-
ferent intersecting angles to form a periodic dielectric array. When these crystals were probed with microwave radiation, they prevented frequencies between 13 and 16 GHz from passing through due to a band gap at these frequency in the periodic array. This means that the pattern of holes creates a band gap, the microwave photons could not propagate internally in any direction. Photons of other frequencies not in the band gaps could pass through. Lawandy took another approach to creating photonic band-gap structures. He built a crystalline structure in a colloidal solution of 100-nm wide polystyrene spheres. Because the tiny spheres are electrically charged, they organize themselves into highly ordered crystals. Then Lawandy embedded light-emitting and light-absorbing dye molecules in the suspension. The dye molecules will emit light after they have been excited by laser light. But the structure of the colloidal crystal blocked their spontaneous emission. After being excited by laser light, the molecules in the suspension did not drop to a lower-energy level and emit photons. Instead, the dye molecules remained excited. This experiment gave further evidence of the effectiveness of periodic dielectric arrays in modifying the propagation of light.

On the other hand, we know that impurities drastically affect the electrical properties of a semiconductor. The addition of boron to silicon atoms increases the conduc-
tivity of pure silicon by a factor of $10^3$ at room temperature.\textsuperscript{11} Also, it affects the band gap in the semiconductor and creates impurity modes in the gap. Does the impurity of dielectric medium affect the photonic band gap as in semiconductors? The addition of a linear dielectric impurity to a periodic dielectric medium will be used in this below to introduce impurity modes in the photonic band gap.

I will create very narrow resonant modes (in frequency) in the gap which have electromagnetic fields localized about the impurity sites. Then I will study the frequency of impurity modes as a function of the dielectric constant between impurity and periodic media and determine what contrasts are needed for an impurity mode to exist.

The first thing I will consider is a periodic system which is formed by an alternating array of $\varepsilon_b$ and vacuum slabs. Using this system I will study the transmission $T$ versus frequency $\omega$ to find band gaps. Then one impurity $\varepsilon_c$ will replace one slab in every $n$-th $\varepsilon_b$ slab to study the transmission versus $\omega$ and find the narrow impurity modes in the gap. For $n>5$, the impurity mode present in the same frequency and this indicated that the general frequency for a single impurity mode is given by our transmission results for $n$-th slab replacements. In this thesis, I will use $n=6$ to do the numerically calculation.

The order of this thesis is as follows: In Chapter II, the introduction of slabs structures and plane wave pro-
pagating through them is given, then I describe the calculation and figures in this study. In Chapter III, I will present all the results in this study.
CHAPTER II

IMPURITY MODES IN PHOTONIC BAND STRUCTURE

I consider the photonic band structure of an impurity system by computing the reflection and transmission of a plane wave incident on such a dielectric medium. The coefficients of reflection and transmission show us the properties of the photonic band structure and its impurity modes. The first thing I consider is a plane wave incident on a single dielectric slab. I will solve for the transmission through the single slab and then use this solution to obtain the transmission through the periodic system with an impurity.

The wave through the single slab is incident from a vacuum dielectric material characterized by a dielectric constant \( \varepsilon_a = 1 \). The slab media is characterized by a dielectric constant \( \varepsilon_b \). Therefore, the structure of a single slab can be described by

\[
\begin{cases}
\varepsilon_a = 1 & \text{if } x \leq x_0 \\
\varepsilon_a = \varepsilon_b & x_0 < x < x_0 + d \\
\varepsilon_a = 1 & x_0 + d < x
\end{cases}
\]

for a slab of thickness \( d \). If a wave propagates in the positive \( x \) direction, the wave can be represented by:
\[ E(x) = Ae^{i(kx - \omega t)}, \]  

(2.2)

where \( A \) is amplitude of the wave, \( k \) is the wave vector in the x-direction and \( \omega \) is frequency of the wave. A general wave through a single slab can be shown to be of the form

\[
E(x, t) = \begin{cases} 
K(A_2 e^{i(k_2 x - \omega t)} + B_2 e^{-i(-k_2 x - \omega t)}) & x \leq x_0 \\
K(A_2 e^{i(k_2 x - \omega t)} + B_2 e^{-i(-k_2 x - \omega t)}) & x_0 \leq x \leq x_0 + d \\
K(A_3 e^{i(k_3 x - \omega t)} + B_3 e^{-i(-k_3 x - \omega t)}) & x_0 + d \leq x 
\end{cases} ,
\]

(2.3)

The complex amplitudes \( A_1, B_1, A_2, B_2, A_3 \) and \( B_3 \) are constants, and \( k_0 \) and \( k \) are the x components of the wave vectors:

\[
k_0 = \frac{\omega}{c} \sqrt{\varepsilon_r} \cos \theta_i, \tag{2.4}
\]

where \( \varepsilon_r \) is dielectric constant, \( \omega \) is frequency and \( \theta_i \) is the ray angle measured from the x axis. Here, we only consider the perpendicular incident wave \((\theta_i = 0)\). Therefore,

\[
k = \frac{\omega}{c} \sqrt{\varepsilon_r} \tag{2.5}
\]

\[
k_0 = \frac{\omega}{c} \sqrt{\varepsilon_r} = \frac{\omega}{c}, \tag{2.6}
\]

The constant \( B_3 \) is the amplitude of the incident wave. The constant \( A_3 \) and \( B_1 \) are amplitudes of the reflected and transmitted waves. Consider the boundary condition at \( x = x_0 \) and \( x = x_0 + d \), we
The $A_3$ is proportional to $k$ and $\omega$. The relation between $A_1$, $B_1$, $A_3$, and $B_3$ can be rewritten to be

$$
\begin{bmatrix}
A_3 \\
B_3
\end{bmatrix} = \frac{1}{4\kappa k_0} \left[ \begin{array}{c}
(k+k_0)^2 e^{i(k-k_0)d} - (k_0-k)^2 e^{-i(k+k_0)d} \\
(k_0-k)^2 e^{i(2k_0x_0+(k-k) d)} + (k^2-k_0^2) e^{i(2k_0x_0+(k-k) d)}
\end{array} \right] \begin{bmatrix}
A_1 \\
B_1
\end{bmatrix} \tag{2.7}
$$

where

$$
\phi = k d = \sqrt{\epsilon k_0} d = \sqrt{\epsilon D}. \tag{2.9}
$$

Assume the plane wave is incident from area III ($x>x_0+d$) through area II to area I ($x<x_0$). Because only the transmitted wave is present in area I, therefore, I set $A_1=0$ and $B_1=1$ to calculate the value of $A_3$ and $B_3$ by eq. (2.8). The transmission coefficient can be written as

$$
t = \frac{B_1}{B_3}. \tag{2.10}
$$

The transmission of wave through the single slab with dielectric media $\epsilon_b$ is given by
A plot of transmission versus frequency for a particular example is shown in Fig.1.

The periodic dielectric structure is formed by a periodic array of slabs. The plane waves which pass through a periodic array of slabs can be treated as a series of single slab transmissions. Therefore, I use a do loop in my computer program to form a periodic array from the single slab solution. The matrix product is solved numerically on computer to find the transmission coefficient for a "periodic" structures using the product of the single slab matrix. I find then the lowest two frequency band gaps and use these to study the photonic gaps problem. The dielectric slabs in the one-dimensional lattice that we use in the studies below were arbitartaken to have $\varepsilon_b = 6$ (Fig.2) or 4 (Fig.3). (Most of dielectric material have $1 < \varepsilon < 10$.) The result for the periodic arrays are presented giving transmission $T$ verse frequency $\omega$ in Figure 2 and 3. The lower energy gaps open in different frequency region for $\varepsilon_b = 4$ and $\varepsilon_b = 6$. At $\varepsilon_b = 6$, we find the lowest three band gaps edges are opened in frequency $0.69 < \omega d/c < 1.08$, $1.59 < \omega d/c < 2.07$ and $2.65 < \omega d/c < 2.85$. At $\varepsilon_b = 4$, the lowest two band gaps opened in frequency $0.84 < \omega d/c < 1.23$ and $1.91 < \omega d/c < 2.30$. 

$$T = |t|^2 = \left| \frac{B_1}{B_2} \right|^2. \quad (2.11)$$
Figure 1. Plot of Transmission $T$ Versus Frequency $\omega$ for Single Dielectric Slab When $\varepsilon_b$=6.
Figure 2. Plot of Transmission $T$ Versus Frequency $\omega$ for Periodic Dielectric Slabs When $\varepsilon_r = 6$. 

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Figure 3. Plot of Transmission $T$ Versus Frequency $\omega$ for Periodic Dielectric Slabs When $\varepsilon_s=4$. 

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Next we put an impurity media in our otherwise periodic array of slabs and calculate the transmission. Specifically, we let the impurity occur by replacing every n-th slab, dielectric media \( \varepsilon_b \), by an impurity \( \varepsilon_c \). The impurity mode is presented in the photonic band gaps as an impurity mode transmission and such transmissions for different values of \( \varepsilon_c \) are shown in Fig. 4 to Fig. 9.

The location of the impurity mode is seen to be related to the dielectric constant of the impurity media \( \varepsilon_c \), relative to its background \( \varepsilon_b \). The frequency of the impurity modes is seen to decrease with increasing impurity dielectric constants as shown in Fig. 10 and Fig. 11. From the impurity modes presented in Fig. 10 and Fig. 11, by replacing an impurity \( \varepsilon_c \) for the background \( \varepsilon_b \), the impurity existed in the lowest band gap of periodic dielectric slab in frequencies \( 0.69 < \omega d/c < 1.08 \) when \( \varepsilon_b = 6 \), and \( 0.84 < \omega d/c < 1.23 \) when \( \varepsilon_b = 4 \). The impurity dielectric constant \( \varepsilon_c \) which creates an impurity mode in the gap is between 0 to 3.4 (\( \varepsilon_c / \varepsilon_b = 0 \) to 0.6) when the background is \( \varepsilon_b = 6 \) and \( \varepsilon_c \) is between 0 to 2.4 (\( \varepsilon_c / \varepsilon_b = 0 \) to 0.6) when the background is \( \varepsilon_b = 4 \).
Figure 4. Plot of Transmission $T$ Versus Frequency $\omega$ for Every 6 Periodic Dielectric Slabs $\varepsilon_b$ Being Replaced by One Impurity $\varepsilon_c$. Here $\varepsilon_b=6$ and $\varepsilon_c=2$. 

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Figure 5. Plot of Transmission T Versus Frequency $\omega$ for Every 6 Periodic Dielectric Slabs $\varepsilon_b$ Being Replaced by One Impurity $\varepsilon_c$. Here $\varepsilon_b=6$ and $\varepsilon_c=2.5$. 

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Figure 6. Plot of Transmission $T$ Versus Frequency $\omega$ for Every 6 Periodic Dielectric Slabs $\varepsilon_b$ Being Replaced by One Impurity $\varepsilon_c$. Here $\varepsilon_b=6$ and $\varepsilon_c=3$. 

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Figure 7. Plot of Transmission $T$ Versus Frequency $\omega$ for Every 6 Periodic Dielectric Slabs $\varepsilon_b$ Being Replaced by One Impurity $\varepsilon_c$. Here $\varepsilon_b=4$ and $\varepsilon_c=2$. 

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Figure 8. Plot of Transmission $T$ Versus Frequency $\omega$ for Every 6 Periodic Dielectric Slabs $\varepsilon_b$ Being Replaced by One Impurity $\varepsilon_c$. Here $\varepsilon_b=4$ and $\varepsilon_c=2.5$. 

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Figure 9. Plot of Transmission $T$ Versus Frequency $\omega$ for Every 6 Periodic Dielectric Slabs $\varepsilon_b$ Being Replaced by One Impurity $\varepsilon_c$. Here $\varepsilon_b=4$ and $\varepsilon_c=3$. 

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Figure 10. Plot of Impurity Mode $\omega$ Versus Impurity Dielectric Constant $\varepsilon_c$ When $\varepsilon_b=6$.
(Result are shown only for the lowest of energy gap.)
Figure 11. Plot of Impurity Mode $\omega$ Versus Impurity Dielectric Constant $\varepsilon_c$ When $\varepsilon_b=4$.
(Result are shown only for the lowest of energy gap.)
CHAPTER III

CONCLUSIONS

As electrons move in the periodic potential formed by the atoms in a crystal, there is a band structure with band gaps. Also, in periodic optical systems in which no light can propagate in the periodic array there is a photonic band structure. Light with frequencies in the photonic band gaps is totally absent from the system. Spontaneous emission is prohibited if its frequency lies within an optical band gap, and this enhances the performance of many semiconductor devices.

We have used the transmission function to study the impurity modes in a one-dimensional dielectric slab and how these modes affect the propagation of light. We looked at the problem by replacing some of the background by impurity. Also, we found the dependence of impurity modes on impurity dielectric and background dielectric constants.

The numerical relation between the transmission and frequencies of electromagnetic waves was calculated on the computer for a single slab and for a periodic array. The transmission in the studies of the periodic arrays give the lower-upper edges of the band gaps presented in frequencies 0.69-1.08, 1.59-2.07 and 2.65-2.85 when waves propagate
through a periodic array of slabs with dielectric constant is 6. The lower-upper gaps are opened in frequency equal to 0.84-1.23 and 1.91-2.30 when we study propagating through periodic slab with dielectric constant 4.

When an impurity is introduced in the periodic slabs, every n-th \( \varepsilon_b \) slabs is replaced by \( \varepsilon_c \), narrow impurity modes may be present in the band gaps. For \( n>5 \), the impurity mode does not change with increasing \( n \), and this indicates that this is the correct frequency for a single impurity. The frequency at which the impurity mode occurs is found to decrease as the dielectric constant of impurity increases relative to the background medium.

The properties of photonic band gaps play an important role in the future development of electronic devices because they offer the possibility of increasing the efficiency of semiconductor devices. Many semiconductor devices, such as semiconductor lasers, hetrojunction bipolar transistors, and solar cells, are all limited by spontaneous emission. By choosing the particular material the performances of many devices will be strongly increased. In addition, our impurity modes are high quality resonators and narrow band gap filter, they will be useful for some specific devices employing these frequency needs. These are discussed in some article in Scientific American recently.
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