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BAND STRUCTURE FOR ACOUSTIC WAVES PROPAGATING IN A PERIODIC ELASTIC MEDIA AND IMPURITY MODES ARISING FROM SLAB SUBSTITUTIONS

by

Abdur Rahman

A Thesis
Submitted to the
Faculty of The Graduate College
in partial fulfillment of the
requirements for the
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Abdur Rahman

BAND STRUCTURE FOR ACOUSTIC WAVES PROPAGATING IN A PERIODIC ELASTIC MEDIA AND IMPURITY MODES ARISING FROM SLAB SUBSTITUTIONS

Abdur Rahman, M.A.

Western Michigan University, 1995

In this thesis I study the band structure for acoustic waves propagating in a one-dimensional elastic array which forms a periodic elastic system in which band gaps are opened in the frequency spectrum. Specifically, I study the single impurity problem in this system. An impurity is introduced in the system by replacing one of the acoustic slabs with a new slab of different acoustic medium or by changing the thickness of impurity slab. I study the very narrow (in frequency) impurity modes in the band gaps which are localized about the impurity sites. Then I study the frequency of impurity modes as a function of thickness of impurity slab or impurity impedance, and determine what conditions are needed for an impurity mode to exist. calculations presented in this thesis are based on numerically studying the transmittance of impurity modes into band gap in one-dimensional, periodic arrays of slabs.

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CHAPTER I

INTRODUCTION

When a quantum or a classical wave propagates in a periodic structure in any number of spatial dimensions, the dispersion curves that relate the frequencies of the wave to the wave vector characterizing its propagation possess an infinite number of branches. These branches form bands that are separated by frequency gaps at various points of the Brillouin zones. In some cases an absolute gap occurs, viz. a frequency range in which no waves can propagate that exists for all values of the wave vector in the density of states of the waves propagating through these structures.² In this thesis we will look at these effects in acoustic systems, and in particular I will look at the effects on the frequency gaps of imperfections which tend to destroy the periodicity of the system.

It is well known from solid state physics that electrons in periodic structures are arranged in energy bands separated by forbidden regions in energy for which no wavelike electron orbits will exist. Such forbidden regions are called band gaps and the properties of band gap systems were originally treated in the studies of electrons in crystals. Only recently, has it been shown that the

concepts of band theory for electrons can also be extended to the description of acoustic waves propagating in a periodic elastic media in number of spatial dimensions (1,2 or 3), and that these structures can be of technological importance.^{2, 11} Specifically, such periodic structures, which produce frequency regions in which no waves propagate, can act as frequency filters or stops.

We know that atomic impurities drastically affect the electrical properties of a semiconductor. In electronic semiconductors small amounts of atomic impurities give rise to impurity modes in the band gaps. These impurity modes have a great effect on the electrical, magnetic and optical properties of semiconductors. In fact, many of the properties utilized in semiconductor devices are produced by suitable doping the material to some appropriate impurity contribution. For example, transistors are created by doping donor or acceptor impurities into silicon material to control the conductivity type (n or p material). We shall see in this thesis that similar impurity modes are found in acoustic systems containing elastic impurities. These impurities can significantly change the stop gaps, affecting the transmissivity (transmission co-efficient) as a function of frequencies of the acoustic waves propagating in these acoustic systems.

In this thesis, I am, specifically interested in the propagation of acoustic waves in a one-dimensional periodic

elastic array (layered system, waves propagating perpendicular to slabs, with band gaps). The replacement of a slab in the periodic array by one slab of varying thickness or different elastic material will be used to introduce impurity modes in the acoustic band structure of the periodic system. I will create very narrow (in frequency) impurity modes in the gap which have acoustic waves localized about the impurity sites. Then I will study the frequency of impurity modes as a function of impurity slab thickness or impurity impedance and determine what conditions are needed for an impurity mode to exist.

I will determine the conditions needed to observe acoustic donor and acceptor levels in a one-dimension slab system. I will use the computer to compute the transmissivity of acoustic waves in the impurity system and will obtain the band gaps and impurity modes by studying the frequency dependence of the transmissivity. The impurity modes in the structure being considered here can be achieved theoretically in two ways:

1. By simply introducing another kind of material slab (impurity slab) into the periodic structure of the slab, just like in producing doped semicondutor and electronic devices, we dope donor or acceptor states into the silicon material. We then observe the variation of the acoustic band, and the possible presence of an impurity level in the gap. We will see, (it is the same as in semiconductor)

this impurity will generate states in the band gaps.

2. By changing the thickness of a slab and studying the relation between the frequency of the impurity mode and the impurity slab thickness.

In this thesis I will concentrate on the second way and will consider at least one example of the first way.

Wave propagation in layered media is a subject of considerable interest and importance in several areas. The subject of plane-wave propagation in layered media lies within the general framework of wave propagating in layered media. As a result of its relative simplicity and the application of results from such studies into a multitude of areas, considerable effort has been and continues to be expended on plane-wave problems in one form or another.

Several approaches are available to investigate planewave propagating in layered media. Among these approaches
are included such techniques of summing the reflection and
transmission of wave fields at each boundary, and the use
of transfer matrix methods. Although the former method
provides an appealing decomposition of reflected and transmitted fields from multilayered media in terms of the
reflection and transmission co-efficients of individual
interfaces, the method is tedious for layered elastic
media. In contrast, the transfer matrix approach, though
less appealing from a physical point of view, is ideal from
computational standpoint for either elastic layer or

multiple layer problems.

A number of recent authors have utilized the transfer matrix method to investigate the reflection and transmission of plane waves from elastic plates. These studies have generalized the original formulation of the transfer matrix approach by incorporating attenuation loss factors into the matrix formulation, thus enabling the treatment of multilayered elastic systems. In addition, these studies have shown that excellent agreement is obtained between the analytical predictions based on transfer matrix methods and corresponding experimental results.

The first thing I will consider is a single slab system of copper slab of characteristic impedance $Z=44.5\times10^6$ MKS-rayls surrounded by aluminum slabs of characteristic impedances $Z_0=17.0\times10^6$ MKS-rayls. Using this system I will study the transmission T versus frequency ω of a single slab. I will obtain a 2×2 transfer matrix for the waves propagating through this system. After this I will study the periodic elastic media which is formed by periodic array of slabs in terms of transfer matrices. Then one impurity will replace one slab in every n-th slab of the periodic system to study the transmission versus frequency and find the narrow impurity modes in the gap. This method for computing the impurity modes is known as the supercell method.

CHAPTER II

BAND STRUCTURE FOR ACOUSTIC WAVES PROPAGATING IN A PERIODIC ELASTIC MEDIA AND IMPURITY MODES ARISING FROM SLAB SUBSTITUTIONS

I consider the band structure for acoustic waves propagating in a periodic elastic media by computing the reflection and transmission of a plane longitudnal waves incident perpendicularly on such a media. The coefficients of reflection and transmission show us the properties of the acoustic band structure and impurity modes. The first thing I consider is a plane acoustic wave incident perpendicularly on a single slab system (eqn. 2.1). I will solve for the transmission and reflection through this single slab, obtaining the 2x2 transfer matrix. will then use this solution to write the solution for a periodic array of slabs in terms of a product of single slab transfer matrices. Finally, I will use this solution to obtain the transmission through the periodic system with an impurity, determining the frequencies of the single impurity leaves in the stop bands.

Acoustic of a Single Homogeneous and Isotropic Layer

I consider a plane acoustic wave incident perpendicularly on a single lab system (eqn. 2.1). The single slab

system is a homogeneous, isotropic, and elastic layer (medium II) of characteristic impedance ρ c sandwiched between two semi-infinite media I and III characterized by the characteristic impedance $\rho_0 c_0$. Therefore, the structure of a single slab of thickness d can be described by:³

$$z(x) = \begin{cases} \rho_0 c_0 & x \le x_0 & I \\ \rho c & x_0 \le x \le x_0 + d & II \\ \rho_0 c_0 & x_0 + d \le x & III \end{cases}$$
 (2.1)

Where ρ_0 and ρ are the densities and c_0 and c are the velocities of the wave propagating in the media in positive x-direction respectively. $z_0=\rho_0c_0$ and $z=\rho c$ are the characteristic impedances of the media, which is defined as the ratio of acoustic pressure in a medium to the associated particle velocity:⁵

$$z = p_{\pm}/u_{\pm} = \pm \rho c \Rightarrow u_{\pm} = \pm p_{\pm}/\rho c$$
 (2.2)

A positive sign is for the waves propagating in the positive x-direction and negative sign is for the waves propagating in the negative x-direction.

For a wave propagating in the positive x-direction in the acoustic media, I can represent the wave equation by:5

$$\frac{\partial^2 \mathbf{p}_i}{\partial t^2} = \mathbf{c}^2 \cdot \frac{\partial^2 \mathbf{p}_i}{\partial x^2} \tag{2.3}$$

Where p_i is the acoustic pressure and c_i is the velocity of the propagation of the wave in the i-th medium.

The solution of eqn. (2.3) gives the wave propagation in the positive x-direction:⁵

$$p_i=Ae^{i(\omega t-kix)}$$
 (2.4)

Where A is the amplitude of the wave, $k_i=\omega/c_i$ is the wave vector in the x-direction and ω is the frequency of the wave.

A general acoustic wave through a single slab propagating in positive x-direction can be shown to be of the form:

Where complex amplitudes A_1 , B_1 , A_2 , B_2 , A_3 and B_3 are constants.

In order to obtain the 2×2 transfer matrix describing acoustic wave propagating through the single slab system, I apply the following two boundary conditions at $x=x_0$ and $x=x_0+d$:

- 1. The continuity of pressure on the two sides of the boundary, i.e. the acoustic pressures on the two sides of the boundary are equal.
- 2. The continuity of the particle velocity on the two sides of the boundary, i.e. the particle velocities normal to the interface are equal.

Therefore, considering the boudary conditions at $x=x_0$ and solving for the relation between A_2 , B_2 and A_1 , B_1 , I have:

$$\begin{bmatrix} A_{2} \\ B_{2} \end{bmatrix} = 1/2z_{0} \begin{bmatrix} (z_{0}+z) e^{i(k-k0)x0} \\ (z_{0}-z) e^{-i(k+k0)x0} \end{bmatrix}$$

$$(z_{0}-z) e^{i(k+k0)xd} \begin{bmatrix} A_{1} \\ B_{1} \end{bmatrix}$$

$$(2.6)$$

Where $z_0 = \rho_0 c_0$ and $z = \rho c$

Similarly, at $x=x_0+d$ I have:

$$\begin{bmatrix} A_{3} \\ B_{3} \end{bmatrix} = 1/2z \begin{bmatrix} (z_{0}+z) e^{-i(k-k0)(x0+d)} \\ -(z_{0}-z) e^{-i(k-k0)(x0+d)} \end{bmatrix} \begin{bmatrix} A_{2} \\ B_{2} \end{bmatrix}$$

$$(2.7)$$

Now combining eqn. (2.6) and eqn. (2.7), I get the required 2×2 transfer matrix:

$$\begin{bmatrix} A_{3} \\ B_{3} \end{bmatrix} = 1/4 z_{0} z \begin{bmatrix} (z_{0}+z)^{2} e^{-i(k-k0)d} - (z_{0}-z)^{2} e^{i(k+k0)d} \\ (z^{2}_{0}-z^{2}) e^{i((k-k0)d-D)} - (z^{2}_{0}-z^{2}) e^{-i((k+k0)+D)} \end{bmatrix}$$

$$(z_{0}^{2}-z^{2}) e^{-i((k-k0)d-D)} - (z_{0}^{2}-z^{2}) e^{i((k+k0)d+D)}$$

$$(z_{0}+z)^{2} e^{i(k-k0)d} - (z_{0}-z)^{2} e^{-i(k+k0)d}$$

$$\begin{bmatrix} A_{1} \\ B_{1} \end{bmatrix}$$

$$\begin{bmatrix} A_{3} \\ B_{3} \end{bmatrix} = \tau (x_{0}, x_{0}+d) \begin{bmatrix} A_{1} \\ B_{1} \end{bmatrix}$$

$$(2.8)$$

Where $D=2k_0x_0$

I assume that the plane wave is incident from area-III $(x \ge x_0 + d)$ through area II $(x_0 \le x \le x_0 + d)$ to area I $(x \le x_0)$. Because only the transmitted wave is present in area I, therefore, I set $A_1=0$ and $B_1=1$ to calculate the values of A_3 and B_3 by eqn. (2.8). The transmission co-efficient can be written as:

$$t=B_1/B_3=1/B_3$$
 (2.9)

The transmission of the wave through the single slab is given by:

$$T=|t|^2=|B_1/B_3|^2=|1/B_3|^2$$
 (2.10)

By changing the frequency ω of the incident wave, I get the relation between transmittance T and frequency ω for a single slab system. The calculations of matrix and transmittance for different ω are completed on vax PDP-11 with FORTRAN program. Figure 1 shows the plot between ω and T when Z=44.5×10⁶ MKS-rayls (Cu) and Z₀=17.0×10⁶ MKS-rayls (Al) (Appendix: Table I⁵), this graph shows that for a single slab system the transmittance is a continuous function of frequency.

Acoustic of One-Dimensional Periodic Structure

The one-dimensional periodic 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.

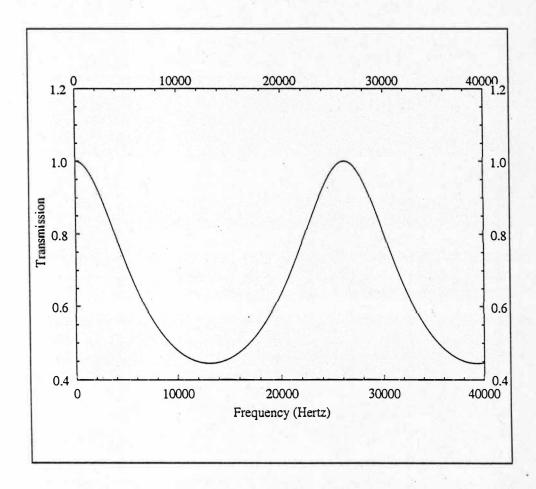


Figure 1. Plot of Transmission T Versus Frequency ω for a Single Slab When Z=44.5x10 6 rayls (Cu), and Z $_0$ =17.0x10 6 rayls (A1).

As in the single slab problem, a plane wave is incident from the right on the periodic structure along x-axis. Passing through the periodic acoustic structure, it finally arrives in area I. I still select $A_i=0$ and $B_i=1$, then the product matrix is given by:

$$\tau (\text{Total}) = \prod_{i=1}^{N} \tau (\text{nd}, (n+1)d)$$

$$n=1$$

$$\begin{bmatrix} A_{i} \\ B_{j} \end{bmatrix} = \tau (\text{Total}) \begin{bmatrix} A_{i} \\ B_{i} \end{bmatrix}$$
(2.11)

The transmittance is given by:

$$T = |1/B_n|^2$$
 (2.12)

To achieve this kind of structure theoretically, in my FORTRAN computer program, I simply use a DO loop to let one slab structure (eqn. 2.1) be repeated for n-times. this, a periodic structure is obtained. The transmittance is solved numerically on computer by calculating a matrix product using the product of single slab matrices. the data, by changing the frequency of the incident wave, I get T versus ω plots for n=6 slabs with slab thickness d=1.0 cm, when Z=39.0×10⁶ MKS-rayls (Ag), Z_0 =17.0×10⁶ MKSrayls (Al) and $Z=44.5\times10^6$ MKS-rayls (Cu), $Z_0=17.0\times10^6$ MKSrayls (Al) (Figures 2 and 3). From these graphs, it is very clear that the transmittance T is no longer a continuous function of frequency ω . The lowest two band gaps are opened in frequencies with 1.10×10^4 Hertz < ω < 1.625×10^4 Hertz and 2.425×10^4 Hertz < ω < 3.125×10^4 Hertz $Z=39.0\times10^6$ MKS-rayls (Ag), $Z_0=17.0\times10^6$ MKS-rayls (Al). $Z=44.5\times10^6$ MKS-rayls (Cu), $Z_0=17.0\times10_6$ MKS-rayls (Al), the band gaps are opened at 1.225×10^4 Hertz < ω < 2.125×10^4 Hertz and 3.025×10^4 Hertz < ω < 3.825×10^4 Hertz.

Impurity Modes in a One-Dimensional Periodic Acoustic Band Structure

When the perfect periodic structure of the one-

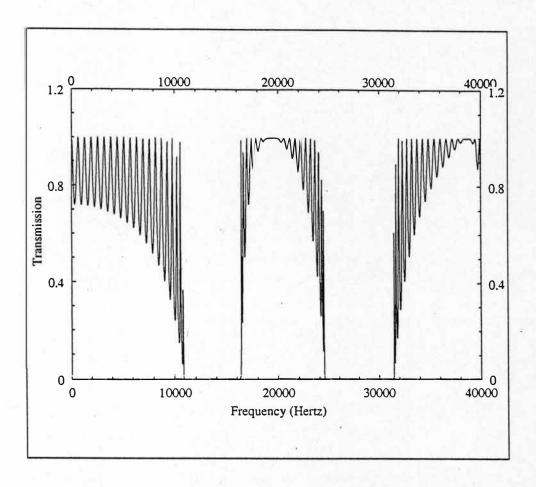


Figure 2. Plot of Transmission T Versus Frequency ω for Periodic Structure When Z=39.0x10⁶ rayls (Ag) and Z₀=17.0x10⁶ rayls (Al).

dimensional array of slabs is disrupted, impurity modes can exist in the band gaps. I put an impurity in my periodic array of slabs and calculate the transmission. Specifically, I let the impurity occur by replacing every n-th slab by an impurity slab.

In a first study, I start with a periodic array of copper and brass layers, each of thickness d=1.0 cm. With the background medium of impedance Z=44.5×10⁶ MKS-rayls (Cu), after every 6 slabs, I change the thickness of one of

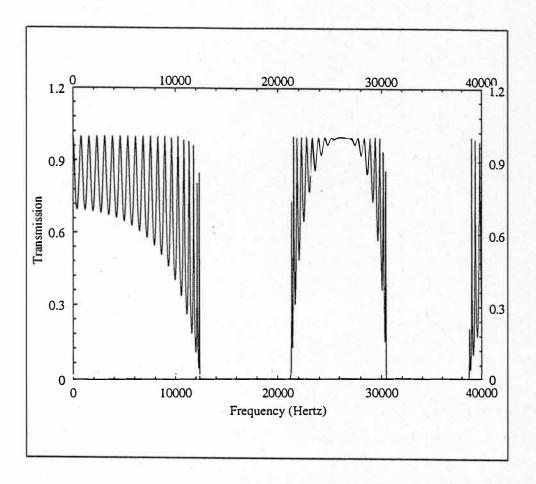


Figure 3. Plot of Transmission T Versus Frequency ω for Periodic Structure When Z=44.5x10⁶ rayls (Cu) and Z₀=17.0x10⁶ rayls (Al).

the slabs with $Z_c=40.0\times10^6$ MKS-rayls (brass) to xd, where $0.0 \le x \le 1.0$ cm, and its right adjacent copper slab to d+(1-x)d, and study the relation between transmission T and frequency ω (Figure 4 to Figure 7).

In a second study, I consider a periodic array of steel and aluminum slabs of thickness d=1.0 cm. After every 6 periodic slabs of impedance Z=47.0×10 6 MKS-rayls (steel), I replace one slab by an impurity slab with impedance Z_c and the same thickness as the original slab and

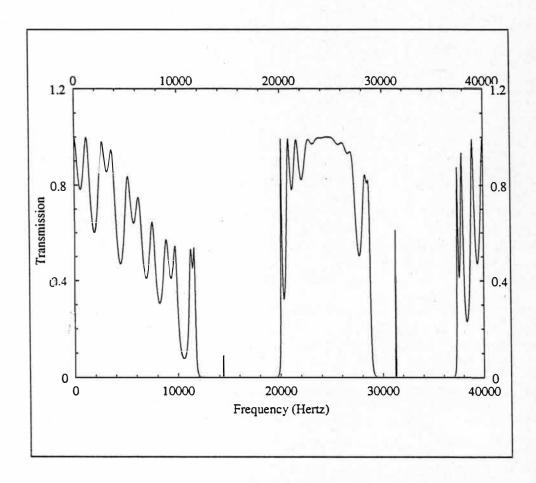


Figure 4. Plot of Transmission T Versus Frequency ω for Periodic Structure With Impurity Size Imperfection When $Z_c=40.0x10^6$ rayls (Brass), x=0.0.

again study the relation between T and ω . Here $Z_c=12.9\times10^6$ MKS-rayls (glass), and $Z_c=23.2\times10^6$ MKS-rayls (Pb), (Figure 8 and Figure 9).

In Figure 10, I present the relation between impurity mode ω_c and the thickness of the impurity slab x in the copper-brass system. Similarly, in Figure 11, I show the results for the relation between the impedance of the impurity slab Z_c relative to the background impedance Z_c

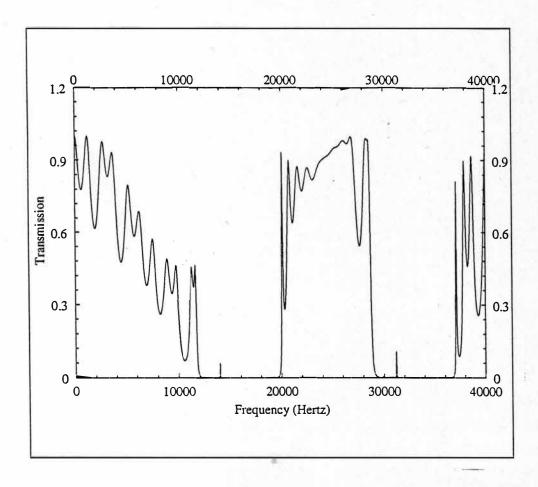


Figure 5. Plot of Transmission T Versus Frequency ω for Periodic Structure With Impurity Size Imperfection When $Z_c=40.0\times10^6$ rayls (Brass), x=0.1 cm.

i.e. Z_c/Z and impurity mode ω_c . These graphs show that the frequency at which the impurity mode occurs decreases as the impurity slab thickness increases or the impedance of the impurity slab relative to background medium increases.

In Figure 10, the thickness of the impurity slab $Z_c=40.0\times10^6$ MKS-rayls (brass) is increased from x=0.0 to 1.0 cm, and its right adjacent background medium Z=44.5×10⁶ MKS-rayls (Cu) to d+(1-x)d. It is observed that as the thickness x is increased the frequency at which the impurity

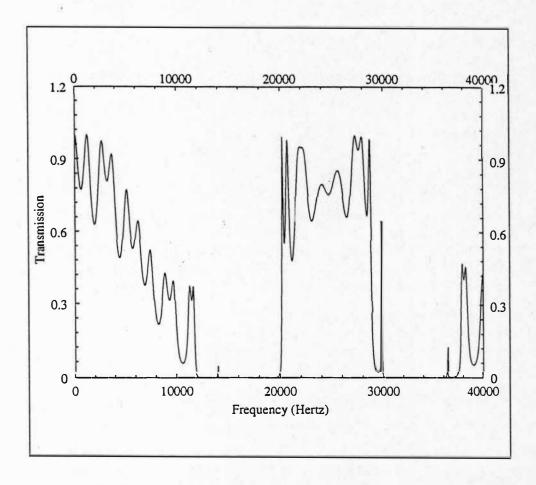


Figure 6. Plot of Transmission T Versus Frequency ω for Periodic Structure With Impurity Size Imperfection When $Z_c=40.0\times10^6$ rayls (Brass), x=0.2 cm.

mode occurs, decreases. It is shown by the Figure 10, which is a plot of impurity thickness x versus impurity mode ω_c .

In Figure 11, every 6 periodic slabs with impedance $Z=47.0\times10^6$ MKS-rayls (steel) is replaced by one impurity slab Z_c . Here $Z_c=12.9\times10^6$ MKS-rayls (glass), and $Z_c=23.2\times10^6$ MKS-rayls (Pb). It is observed that as impedance of impurity slab Z_c relative to background medium's impedance

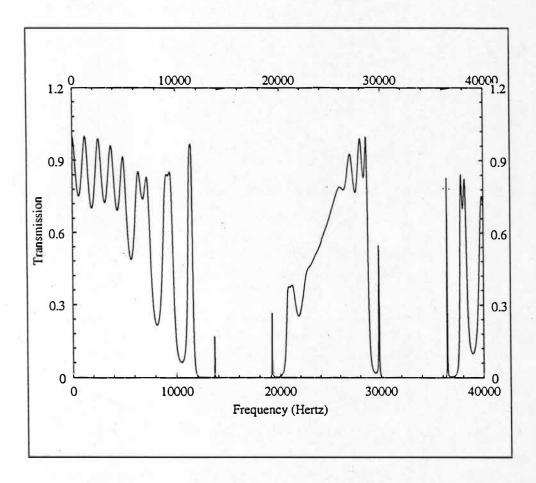


Figure 7. Plot of Transmission T Versus Frequency ω for Periodic Structure With Impurity Size Imperfection When $Z_c=40.0\times10^6$ rayls (Brass), x=0.7 cm.

Z, i.e. Z_c/Z , is increased, frequency at which the impurity mode occurs, decreases. It is shown by Figure 11, which is a plot of impurity mode ω_c versus Z_c/Z .

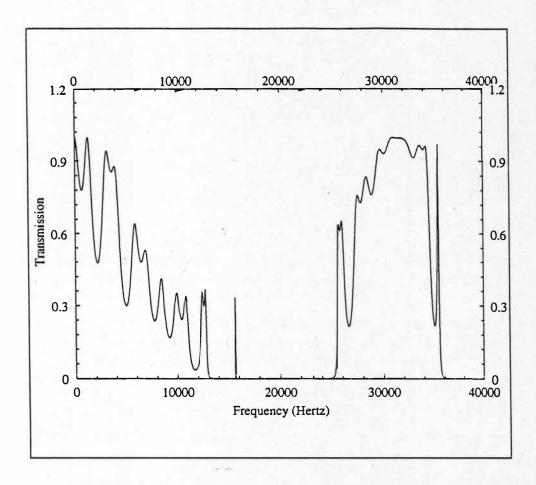


Figure 8. Plot of Transmission T Versus Frequency ω for Periodic Structure With Impurity Replacement. Here $Z_c=12.9\times10^6$ rayls (Glass).

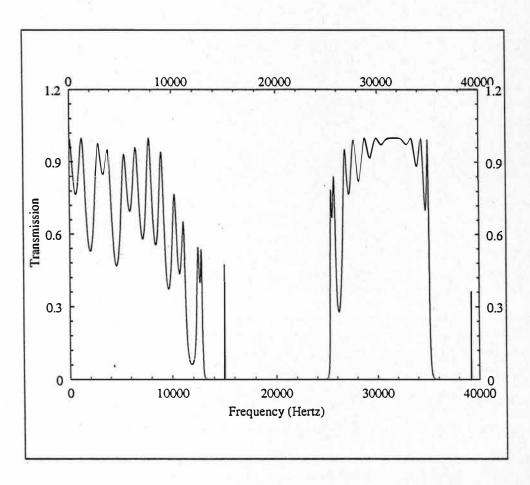


Figure 9. Plot of Transmission T Versus Frequency ω for Periodic Structure With Impurity Replacement. Here $Z_c = 23.2 \times 10^6$ rayls (Pb).

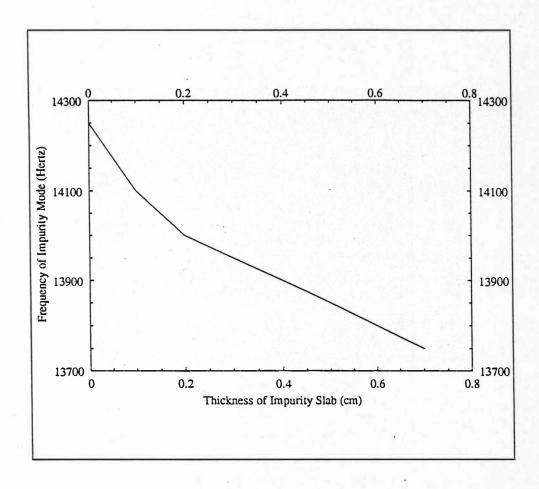


Figure 10. Plot of Frequency of Impurity Mode ω_c Versus Thickness of Impurity Slab x When $Z_c=40.0x10^6$ rayls (Brass) and $Z=44.5x10^6$ rayls (Cu).

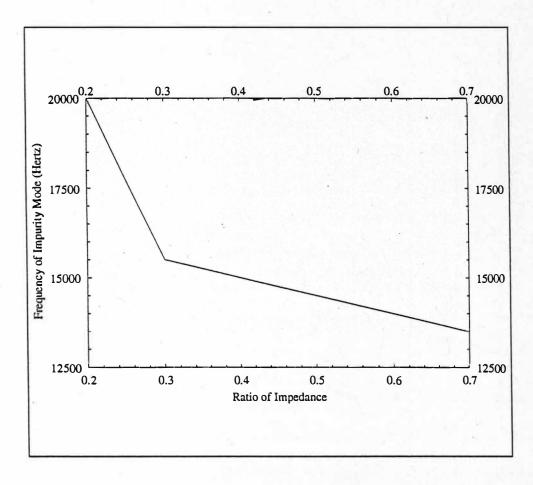


Figure 11. Plot of Frequency of Impurity Mode ω_c Versus Ratio of Impedance Z_c/Z When $Z=47.0\times10^6$ rayls (Steel).

CHAPTER III

CONCLUSIONS

According to the band theory in solid state physics, electrons in periodic crystals are arranged in energy bands separated by band gaps. Similarly, this band theory can also be employed to explain the propagation of acoustic waves in a periodic structures in any number of spatial dimensions. Acoustic waves with frequencies falling in the acoustic band gaps are totally absent from the system. Similarly, as with donor or acceptor impurities in n-type or p-type semiconductor materials, impurity modes can also be introduced into the acoustical band structures by replacing some of the material of the media with impurity material of a different characteristic impedance or size. These impurity modes in the acoustic system are then localized vibration modes in the structures and are bound to the site of the impurity material.

In Chapter II, I have discussed the propagation of acoustic waves through a single slab system, one-dimensional periodic structure consisting of an array of parallel slabs, and also through the periodical system with a single impurity. The transmission function versus the frequencies of acoustic waves was calculated in all these

cases. From these graphs, I see that, for the periodic arrangement of the slabs, the transmittance is no longer a continuous function of frequency, as in the single slab case, but instead, there are band gaps in the dispersion curves. The lower-upper edges of the first two band gapes are present in frequencies 1.10×10^4 Hertz < ω < 1.625×10^4 Hertz and 2.425×10^4 Hertz < ω < 3.125×10^4 Hertz for slab with Z=39.0×10⁶ MKS-rayls (silver) and Z=17.0×10⁶ MKS-rayls (Al). For Z=44.5×10⁶ MKS-rayls (Cu), Z₀=17.0×10⁶ MKS-rayls (Al) the band gaps are at frequencies 1.225×10^4 Hertz < ω < 2.225×10^4 Hertz and 3.025×10^4 Hertz < ω < 3.825×10^4 Hertz. In addition, the introduction of impurities in these periodic structures is found to introduce additional impurity modes in the band gaps.

When an impurity is introduced in the periodic structure, every n-th Z slabs is replaced by an impurity slab $z_{\rm c}$ or the impurity slab thickness is changed, narrow impurity modes may be present in the band gaps. The frequency at which the impurity mode occurs is found to decrease as the impurity slab thickness increases or the characteristic impedance of impurity relative to the background medium increases.

The properties of acoustical band structure and the localized impurity mode in the band gaps can be very useful in the improvement of many acoustic devices. By creating

some kind of impurity disorder into the perfect periodic structure, impurity modes can be introduced into the acoustical band gap at some particular frequencies. This kind of structure can be used as narrow band filters, isolators, and as high quality resonators.

All the impurity modes studied in our work are linear impurities. Future work in this area can be done in the area of acoustic wave propagating in one-dimensional periodic structures with non-linear impurities. In such material the characteristic impedance of the impurity slab is a function of the intensity of the acoustic wave.

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