Studies on Dispersion Behavior of Phonons in AlN/GaN/AlN Heterostructure

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MASTER OF SCIENCE in

PHYSICS

Submitted by

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Certificate

I hereby certify that the work which is being presented in the thesis entitled, **"Studies on Dispersion Behavior of Phonons in AlN/GaN/AlN Heterostructure"**, in partial fulfillment of the requirements for the award of degree of Master of Physics submitted in School of Physics and Material Science of Thapar University, Patiala, is an authentic record of my own work carried out under the supervision of Dr. Dwijendra Pratap Singh and refers other researcher's works which are duly listed in the reference section.

The matter presented in this thesis has not been submitted for the award of any other degree of this or any other university.

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This is to certify that the above statement made by the candidate is correct and true to the best of my knowledge.

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ABSTRACT

Dispersion relation of a material is of general importance in predicting its electronic structure, thermal behavior and optical properties. It becomes quite important in low dimension systems such as nanostructure (quantum dot, nanowire and thin film) and heterostructure. Because, in the low dimensional systems, understanding of propagation of phonon is of quite importance as it is responsible for change in various physical properties. Therefore reduction of problem to elastic continuum model and MATLAB programming has carried out for GaN free standing nanostructure and AlN/GaN/AlN heterostructure. The dispersion behavior for the free standing GaN has been found to be anomalous as compared to its bulk counterpart. The difference in the dispersion of GaN free standing nanostructure and AlN/GaN/AlN heterostructure has also been noticed. The difference might be coming due to changed nature of phonon waves at the interfaces. The variation of group velocity with propagation constant has also been studied. Again the different behavior of bulk sample, free standing nanostructure and nanostructure has been found.

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Chapter 1
Introduction

1.1 Introduction

The quantization of lattice vibration called as phonon has been used for explaining the specific heat behavior of metal and insulators [1] [2]. The relation between the frequency of phonon and its propagation constant is called as dispersion relation. The dispersion relation of material has been utilized for explaining the various physical properties. These physical properties are electronic structure (band gap, densities of states etc.), thermal properties, optical properties etc. more recently the various semiconductors and their heterostructure has been used for various devices [3][4][5]. Whenever a heterostructure is being utilized for device fabrication, then the heat evolution or dissipation at the interface and thermal conduction across interface plays an important role. In the low dimensional system such as free standing nanostructure and heterostructure, the phenomenon of thermal transport is quite interesting [6]. Thermal transport behavior can be easily understood by having knowledge of dispersion relation. Phonon dispersion relation is strongly modified in freestanding thin films or in nanostructures embedded into elastically dissimilar materials. Such modification may turn out to be desirable for some applications while detrimental for others. For example such modification resulting in high thermal conductivity is beneficial to heat evacuation in modern ICs, on the other hand low thermal conductivity is preferred for thermoelectric devices [7].The subsequent section of this chapter briefly explains the importance of dispersion relation in predicting different physical behavior.

Broadly we can say that phonon dispersion can be tuned to control the following properties of heterostructure or nanostructures:

- Thermal properties.
- Electrical properties.
- Optical properties.

1.1.1 Thermal properties: The thermal properties of semiconductor nanostructures have attracted significant attention due to the continuous shrinking feature dimensions of microelectronic devices [8][9][10][11]. Dispersion relation is important in understanding the following thermal properties of a structure:

- Specific heat.
- Thermal conductivity.
- Thermal expansion.

1.1.1.1 Specific heat

Specific heat is the amount of thermal energy required to raise the temperature of a unit mass of a material by one degree. The rise in temperature of material, when it is heated is attributed to the increase in total internal energy of the material. This total internal energy has contribution mainly from

i. Lattice vibrations.
ii. Kinetic energy of free electrons.

When talking about semiconductors, contribution due to free electrons is negligible as the semiconductors have very less number of free electrons (provided it is lightly doped). The first quantum theory of lattice specific heat for a non-metallic solid was given by Einstein. This theory is able to explain qualitatively the temperature dependence of specific heat of solids but not at low temperate. A relatively correct theory was given by Debye. In this theory Debye assumed the solid to be a continuous medium ignoring the discrete structure of crystal lattice and considered the equation of stationary waves in a cubic solid.

Considering one dimensional structure of length L, the periodic boundary condition for stationary elastic wave in x direction is

$$\exp(ikx) = \exp[ik(x + L)]$$

Where *k* is the wave vector of the phonon. The above boundary condition leads to the possible values of *k* as

$$k = 0, \pm\frac{2\pi}{L}, \pm\frac{4\pi}{L} \dots\dots\dots$$

Thus the number of modes in one dimension is $L/2\pi$. Similarly in three dimension the density of modes will be $(L/2\pi)^3$. The number of modes in the range k to k+dk

$$D(k)dk = \left(\frac{L}{2\pi}\right)^3 4\pi k^2\, dk$$

Total number of modes with wave vector less than *k* can be found by integrating the above equation from 0 to *k*. Thus for each polarization type

$$N = \left(\frac{L}{2\pi}\right)^3 \frac{4\pi k^3}{3}$$

The density of states for each polarization is

$$D(\omega) = \left(\frac{Vk^2}{2\pi^2}\right)\frac{dk}{d\omega}$$

Or

$$D(\omega)d\omega = \left(\frac{Vk^2}{2\pi^2}\right)\frac{d\omega}{d\omega/dk}$$

Once the dispersion relation is known, the numbers of modes in the frequency range ω to ω+dω can be calculated (Debye in his theory of lattice specific heat assumes a simple dispersion relation $\omega=v_s k$ [12]). From which total internal energy and hence the specific heat can be calculated.

1.1.1.2 Thermal conductivity

The most important thermal property affected by the phonon dispersion due to phonon confinement is thermal conductivity [6][13][14]. Effect of phonon dispersion on thermal conduction across Si/Ge interface has been studied by D. Singh, J. Y. Murthy and T. S. Fisher through the simulation of phonon Boltzmann transport equation [15].

Heat in technologically important semiconductors is carried out by acoustic phonons. When the size of heterostructure or nanostructure is decreased then the thermal conductivity can decrease for two basic reasons [16]. The first is the co-called classical size effect on thermal conductivity related to the increased phonon-rough boundary scattering. This effect is pronounced when size is of the order of phonon mean free path. It can be observed even in bulk samples at sufficiently low temperature when the phonon mean free path is long. Secondly when the structure dimensions is considerably less than mean free path, a more interesting effect takes place. Due to flattening of the dispersion branches, the population average phonon group velocity decreases leading to the increased phonon scattering on defects or interfaces. As a result, the in-plane thermal conductivity in freestanding thin films

or nanowires can be significantly reduced. As one can see in Figure 1.1, acoustic phonon confinement leads to the reduction of the thermal conductivity from its bulk value even in a nanowire with ideally smooth surface [17]. The straight line is showing the thermal for bulk structure.

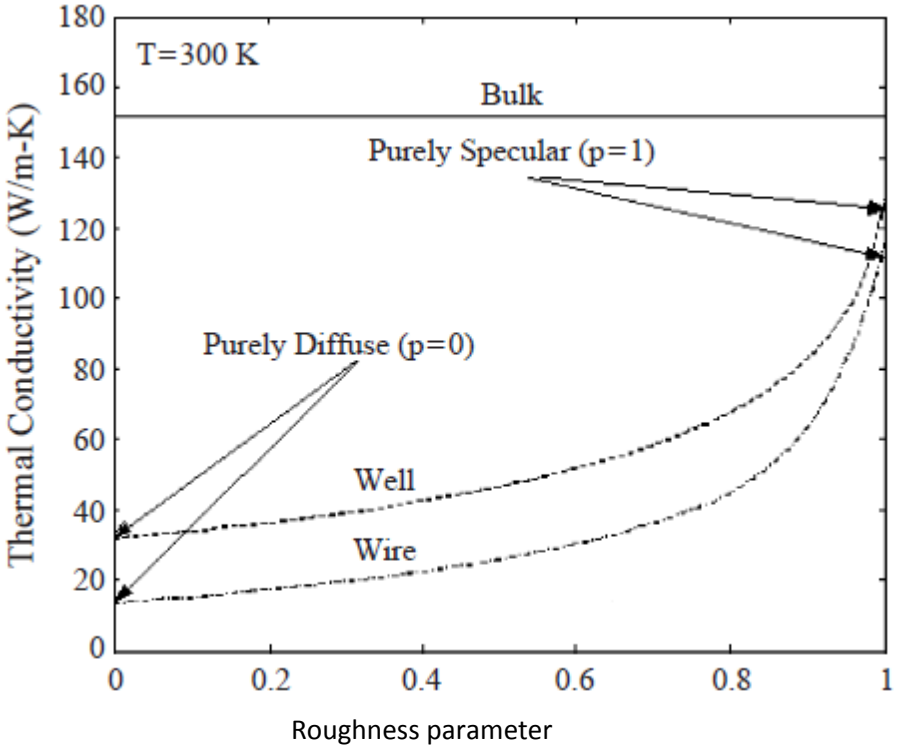

Figure 1.1: Variation of Thermal conductivity with Roughness Parameter. p=1 corresponds to purely smooth surface.

On the other hand thermal conductivity can be increased by embedding nanostructures into "acoustically faster" or "acoustically harder" barrier (cladding) layers [13].

1.1.1.3 Thermal expansion

Thermal expansion is a measure of the increase in length of the material due to rise in temperature. Expansion of solids on heating is a direct consequence of anharmonicity of the vibrations of the atoms in the lattice [12]. For nanostructures coefficient of thermal expansion become very important due to its variation with size. It has been predicted that the fractional change in the Coefficient of Thermal Expansion from the bulk value scales inversely with the size of the nanostructure [18]. Thermal expansion of a material can be

expressed in terms of Gruneisen parameter which can be calculated for all the phonon modes by a linear fit to the dispersion curve [19]. The Gruneisen parameter expresses the volume dependence of the mode frequency and is defined for mode‘s’ and wave vector ‘k’ as

$$\gamma_{s,k} = -\frac{V}{\omega_{s,k}} \frac{\partial \omega_{s,k}}{\partial V}$$

The thermal expansion coefficient itself can be written in terms of Gruneisen parameter as

$$\alpha = \frac{1}{BV} \sum_{s,k} \hbar \omega_{s,k} \gamma_{s,k} \frac{\partial n_{s,k}}{\partial T}$$

Where B is the bulk modulus and $n_{s,k}$ is the phonon occupation number. Gruneisen parameter is positive for positive thermal expansion and negative for negative thermal expansion [20][21].

1.1.2 Electrical properties: Dispersion relation is important in understanding the following electrical properties of a structure:

- Electrical conductivity.
- Carrier mobility
- Band gap (of Heterostructure or quantum well).
- Electronic structure.

1.1.2.1 Electrical conductivity

Electrical conductivity is the measure of ability of material to conduct an electrical current. Electrical conductivity can be modified by using the phonon depletion in acoustically mismatched nanostructures [22]. Spatial confinement of acoustic phonons in nanoscale structures with the large mismatch of the acoustic impedances at the interfaces can strongly affect the phonon spectrum and substantially modify the electron–phonon interaction in comparison with bulk. In such structures, both confinement of electron states and acoustic phonons should be taken into account while calculating the scattering rates. In the reference 22 it has been theoretically shown that the phonon population in thin films or nanowires embedded into acoustically softer materials can be depleted, and the carrier-phonon scattering rate is suppressed.

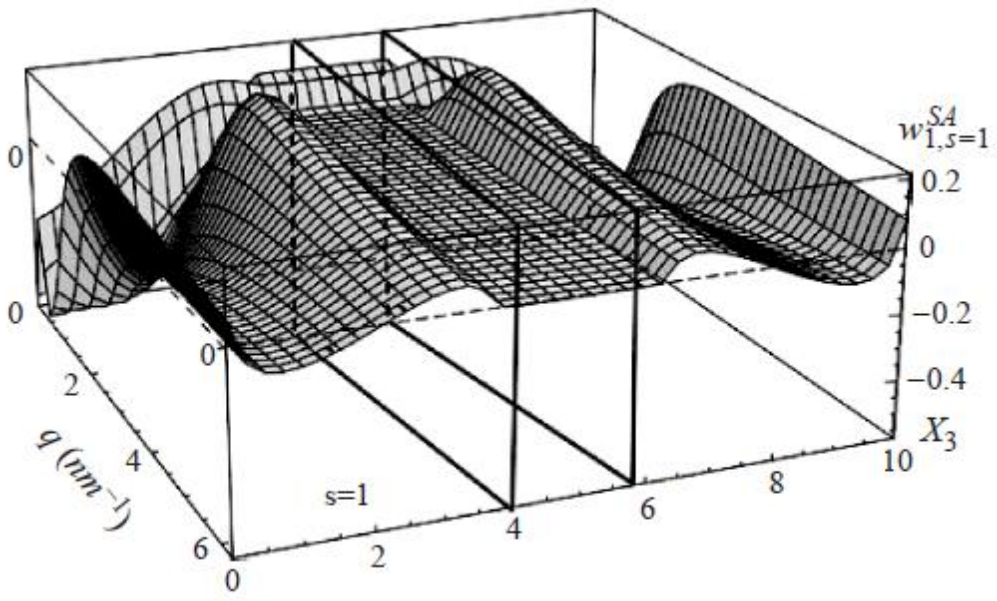

Figure 1.2: Depletion of Phonons from the core layer.

Note that the displacement component surfaces are nearly flat and close to zero inside the core layer of the heterostructure while the amplitudes of vibrations are high in the cladding layers. This effect can be used to suppress the inelastic scattering in nanowires and increase electrical conductivity.

1.1.2.2 Carrier mobility

Mobility is a measure of how easily a carrier moves in a particular material. It is defined as the ratio of carrier velocity in the field direction to the magnitude of the electric field. In semiconductor, carrier mobility applies to both electrons and holes. Relation between the carrier mobility and effective mass can be given as

$$\mu = \frac{|e|\tau}{m^*}$$

Where e is charge on carrier, τ is relaxation time and m is the mobility of the carrier. So the mobility varies inversely with effective mass. The effective mass of a charge carrier can be expressed as

$$m^* = \frac{\hbar^2}{(d^2E/dk^2)}$$

That is the effective mass varies inversely with the slope of group velocity versus wave vector curve. Thus dispersion relation provides important information about effective mass and charge carrier mobility. A mobility enhancement of 2 times and 100 times has been observed at room temperature and at 10K respectively in silicon nanowires by embedding the nanowires into acoustically harder material such as diamond [23]. Since diamond is a good heat conductor the mobility enhancement is accompanied by an extra benefit of improved thermal management.

1.1.3 Optical properties

Dispersion relation is also important in predicting the optical properties of materials. The Kramers-Kronig relation utilizes the ω-k relationship and predicts the refractive index and change in real and imaginary part of dielectric function [24]. This type of study has been carried for explaining the electronic structure and optical properties of α-MnSe [25]. Application of dispersion relation for optical properties has also been reported elsewhere [26][27].

1.1.4 Aim of the thesis

Previous sections of this chapter emphasize the importance of dispersion relation in predicting physical properties. Particularly semiconductor heterostructures [6] and low dimensional metallic structures [28] are of immense importance. Therefore the result in the present thesis is aimed at

1. MATLAB programming for obtaining dispersion behavior of acoustical phonon in free standing GaN nanostructure.
2. MATLAB programming of obtaining dispersion behavior of AlN/GaN/AlN heterostructure.
3. To study the change in dispersion behavior of phonons and their group velocities in varying thickness heterostructure.

Chapter 2
Numerical Methodology

2.1 Introduction

The first chapter puts light on the dispersion of phonons in materials and its significance. This chapter provides a numerical approach to get the dispersion relation in a free standing and embedded nanostructure, which relies on general elastic mechanics to investigate the phonons in these structures. Such treatment has received great successes in semiconductor quantum dot [29], nanotubes [30], semiconductors nanofilms [31], and metallic nanofilms [28]. The phonon dispersion relation has been solved in the elastic continuum approximation. Starting with the equation of motion for the elastic medium a solution in the form of sinusoidal traveling waves has been assumed. This is subjected to appropriate boundary conditions. The problem has been then reduced to numerical problem by using the Newton finite difference formula. The reduced problem is in fact a system of linear homogeneous equations, which is further reduced to an Eigen value problem with Eigen values as square of angular frequency.

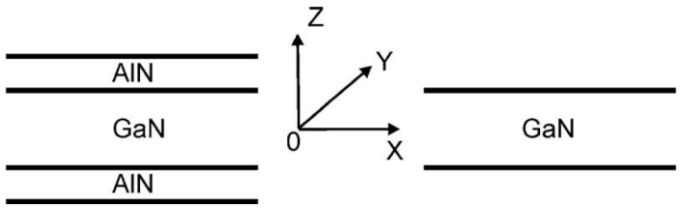

Figure 2.1: Schematics of a free-standing AlN/GaN/AlN heterostructure (left) and a free standing GaN thin film (right). The coordinate system is shown in the middle. The z direction is confined in both the cases.

2.2.1 Problem Definition

The schematic of the problem is shown above in the figure 2.1. A shear wave travelling along the X axis will be considered such that the motion of particles is along Y axis. Z

direction is confined only to few nanometers. The origin of the axis lies in the centre of the heterostructure. If 't' is the total thickness of the heterostructure along Z axis, then its ends lies at z=-t/2 and z=z/2

2.2.2 Problem Reduction

Differential equation for a shear wave travelling in x direction such that particle displacement is along y axis [24] is

$$\rho \frac{\partial^2 U_y}{\partial t^2} = \frac{\partial Y_x}{\partial x} + \frac{\partial Y_y}{\partial y} + \frac{\partial Y_z}{\partial z} \qquad \text{---------- (1)}$$

Where the Y_x, Y_y and Y_z are the stress components, ρ is density and U_y is the y component of the displacement vector. If deformations are small then according to Hooks law, the stress components are linearly related to the strain components and the coefficients are called the elastic stiffness constants. In a hexagonal crystal, such as wurtzite GaN, the independent elastic stiffness constants are C_{11}, C_{12}, C_{13}, C_{33}, C_{44}, and C_{66}. In heterostructure AlN/GaN/AlN the density ρ and stiffness constants C_{ij} are defined as

$$\rho(z) = \begin{cases} \rho_{AlN} & -\frac{t_{GaN}}{2} - t_{AlN} \le z < -\frac{t_{GaN}}{2} \\ \rho_{GaN} & -\frac{t_{GaN}}{2} \le z < \frac{t_{GaN}}{2} \\ \rho_{AlN} & \frac{t_{GaN}}{2} \le z \le \frac{t_{GaN}}{2} + t_{AlN} \end{cases} \qquad \text{--------- (a)}$$

$$C_{ij}(z) = \begin{cases} C_{ij(AlN)} & -\frac{t_{GaN}}{2} - t_{AlN} \le z < -\frac{t_{GaN}}{2} \\ C_{ij(GaN)} & -\frac{t_{GaN}}{2} \le z < \frac{t_{GaN}}{2} \\ C_{ij(AlN)} & \frac{t_{GaN}}{2} \le z \le \frac{t_{GaN}}{2} + t_{AlN} \end{cases} \qquad \text{-------- (b)}$$

Where ρ_{AlN} and ρ_{GaN} are the densities of Aluminum Nitride and Gallium Nitride respectively. t_{AlN} and t_{GaN} are the thickness of Aluminum Nitride and Gallium Nitride slabs in the heterostructure respectively. Similarly $C_{ij(AlN)}$ and $C_{ij(GaN)}$ are the stiffness constants in different directions for Aluminum Nitride and Gallium Nitride respectively.

The solution of equation (1) can be given as

$$U_y = U_y(z) * \exp[i(\omega t - kx)]$$

Where U_y is the amplitude which depends upon z coordinate and k is the x component of the wave vector.

Using this solution in the equation (1) and applying the relation between stress strain and displacement components we can derive the equation for our heterostructure, which is given as a second order differential equation

$$\frac{d^2u_y(z)}{dz^2}+\frac{1}{C_{44}(z)}\frac{dC_{44}(z)}{dz}\frac{du_y(z)}{dz}+\frac{1}{C_{44}(z)}[\rho(z)\omega^2-C_{66}(z)k^2]u_y(z)=0 \quad \text{---- (2)}$$

If we consider a single thin film of density ρ and stiffness constants C_{44} and C_{66} then the second term of equation (2) will be zero and differential equation representing the single thin film is

$$\frac{d^2u_y(z)}{dz^2}+\frac{1}{C_{44}}[\rho\omega^2-C_{66}k^2]u_y(z)=0 \quad \text{--------- (3)}$$

The free-standing boundary conditions require that the stress and strain are zero at the surfaces, that is,

$$\frac{du_y(z)}{dz}=0 \text{ at } z=\pm t/2 \quad \text{--------- (4)}$$

Equation (2) with the free-standing boundary conditions cannot be solved analytically and numerical techniques need to be applied. Whereas equation (3) can be solved analytically and gives the solution

$$\omega=\sqrt{\frac{C_{66}k^2+C_{44}k_z^2}{\rho}} \quad \text{---------- (5)}$$

Where k_z is the component of the wave vector in the z direction. Due to the boundary conditions, k_z is quantized and is given by $k_z=n\pi/t$, where n is a positive integer and t is the thickness of the thin film. The quantization of the phonon modes is due to the spatial confinement of phonons, similar to the confinement of an electron in a quantum well.

To solve for the phonon dispersion in a heterostructure numerically, we use a finite difference method. The numerical algorithm takes four steps.

1. Divide the total thickness t of the heterostructure into N equal parts of width $h=t/N$. The z coordinate of each node is given by: $z_i=z_0+ih$, where $z_0=-t/2$, and i=1, 2, ... $N+1$.

   Thus

$$h = \frac{t}{n} = \frac{t_{GaN} + 2t_{AlN}}{n}$$

$$z_i = z_0 + ih = -\frac{t}{2} + ih$$

$$z_i = -\frac{1}{2}[t_{GaN} + 2t_{AlN}] + i[\frac{t_{GaN} + 2t_{AlN}}{n}]$$

This on simplification gives

$$z_i = \frac{[i - \frac{n}{2}]t_{GaN} + t_{AlN}[2i - n]}{n}$$

Thus $\rho(z_i)$, $C_{44}(z_i)$ and $C_{66}(z_i)$ can be calculated for different nodes using *(a)* and *(b)*.

2. From the central difference formula first and second order derivative can be given as

$$\frac{dC_{44}}{dz} = \frac{C_{44,i+1} - C_{44,i-1}}{2h}; \quad \frac{du}{dz} = \frac{u_{i+1} - u_{i-1}}{2h}; \quad \frac{d^2u}{dz^2} = \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2}$$

Substituting these in equation (2) we get

$$\left(\frac{u_{i+1} - 2u_i + u_{i-1}}{h^2}\right) + \frac{1}{C_{44,i}}\left(\frac{C_{44,i+1} - C_{44,i-1}}{2h}\right)\left(\frac{u_{i+1} - u_{i-1}}{2h}\right) + \frac{1}{C_{44,i}}[\rho(z_i)\omega^2 - C_{66,i}k^2]u_i = 0$$

This gives

$$u_{i-1}\left[\frac{C_{44,i-1} + 4C_{44,i} - C_{44,i+1}}{4h^2}\right] + u_i\left[\rho(z_i)\omega^2 - C_{66,i}k^2 - \frac{2C_{44,i}}{h^2}\right]$$

$$+u_{i+1}\left[\frac{-C_{44,i-1}+4C_{44,i}+C_{44,i+1}}{4h^2}\right]=0 \qquad \text{------- (6)}$$

Equation (6) represents *n+1* algebraic equations with *i* =1, 2, . . . , *n+1*, thus forming a system of *n+1* linear homogeneous equations. Equation (6) can be rewritten as

$$u_{i-1}\left[\frac{C_{44,i-1}+4C_{44,i}-C_{44,i+1}}{4h^2}\right]+u_i\left[-C_{66,i}k^2-\frac{2C_{44,i}}{h^2}\right]$$
$$+u_{i+1}\left[\frac{-C_{44,i-1}+4C_{44,i}+C_{44,i+1}}{4h^2}\right]=-u_i\rho(z_i)\omega^2 \qquad \text{--------- (7)}$$

If we apply the free-standing boundary conditions and use the central-difference approximation, we find

$$\left.\frac{du(z)}{dz}\right|_{z=-t/2}\approx\frac{(u_{i+1}-u_{i-1})}{2h}=0 \qquad \text{For i=1, n+1}$$

Which gives $u_2 = u_0$ and $u_{n+2} = u_n$. This will modify the first and last equation of our system as:

$$\frac{2C_{44,1}}{h^2}u_2+u_1\left(-C_{66,1}k^2-\frac{2C_{44,1}}{h^2}\right)=-u_1\rho(z_1)\omega^2 \qquad \text{---------- (8)}$$

$$\frac{2C_{44,n+1}}{h^2}u_n+u_{n+1}\left(-C_{66,n+1}k^2-\frac{2C_{44,n+1}}{h^2}\right)=-u_{n+1}\rho(z_{n+1})\omega^2 \qquad \text{---------- (9)}$$

Equation (7) along with equation (8) and (9) can be written in the matrix form as

$$[A][U]=\lambda[B][U] \qquad \text{---------- (10)}$$

Here

- [*A*] is a (*n+1*) × (*n+1*) matrix as given on next page.
- $\lambda = \omega^2$
- [*U*] is a (*n+1*) × *1* given by

$$[U]=[u_1\, u_2\, u_3\, u_4\, u_5 \ldots\ldots u_{n+1}]^T$$

- [*B*] is a (*n+1*) × (*n+1*) diagonal matrix with its elements equal to $-\rho(z_i)$ as given on second next page.

Matrix A

$$\begin{bmatrix}
\frac{-2C_{44,1}}{h^2} - C_{66,1}k^2 & \frac{2C_{44,1}}{h^2} & 0 & 0 & . & 0 & 0 & 0 \\
\frac{C_{44,1} - C_{44,3} + 4C_{44,2}}{4h^2} & -\frac{2C_{44,2}}{h^2} - C_{66,2}k^2 & \frac{C_{44,3} + 4C_{44,2} - C_{44,1}}{4h^2} & 0 & . & 0 & 0 & 0 \\
0 & \frac{C_{44,2} - C_{44,4} + 4C_{44,3}}{4h^2} & -\frac{2C_{44,3}}{h^2} - C_{66,3}k^2 & \frac{C_{44,4} + 4C_{44,3} - C_{44,2}}{4h^2} & . & 0 & 0 & 0 \\
0 & 0 & \frac{C_{44,3} - C_{44,5} + 4C_{44,4}}{4h^2} & -\frac{2C_{44,4}}{h^2} - C_{66,4}k^2 & . & 0 & 0 & 0 \\
0 & 0 & 0 & \frac{C_{44,4} - C_{44,6} + 4C_{44,5}}{4h^2} & . & 0 & 0 & 0 \\
. & . & . & . & . & . & . & . \\
0 & 0 & 0 & 0 & . & \frac{C_{44,n-1} - C_{44,n+1} + 4C_{44,n}}{4h^2} & -\frac{2C_{44,n}}{h^2} - C_{66,n}k^2 & \frac{C_{44,n+1} + 4C_{44,n} - C_{44,n-1}}{4h^2} \\
0 & 0 & 0 & 0 & . & 0 & \frac{2C_{44,n+1}}{h^2} & \frac{-2C_{44,n+1}}{h^2} - C_{66,n+1}k^2
\end{bmatrix}$$

Matrix B

$$\begin{bmatrix} -\rho(z_1) & 0 & 0 & 0 & . & 0 & 0 & 0 \\ 0 & -\rho(z_2) & 0 & 0 & . & 0 & 0 & 0 \\ 0 & 0 & -\rho(z_3) & 0 & . & 0 & 0 & 0 \\ 0 & 0 & 0 & -\rho(z_4) & . & 0 & 0 & 0 \\ . & . & . & . & . & . & . & . \\ 0 & 0 & 0 & 0 & . & -\rho(z_{n-1}) & 0 & 0 \\ 0 & 0 & 0 & 0 & . & 0 & -\rho(z_n) & 0 \\ 0 & 0 & 0 & 0 & . & 0 & 0 & -\rho(z_{n+1}) \end{bmatrix}$$

Let us define [C] = [B] $^{1/2}$. As [B] is a diagonal matrix [C] will also be a diagonal matrix. Also

$$C_{ij} = B_{ij}^{1/2} \quad or \quad B_{ij} = C_{ij}^2 \quad or \quad [B] = [C]^2$$

--------- (11)

Now Define Matrix P as

$$[P] = [C]^{-1}[A][C]^{-1}$$ ---------- (12)

Or

$$[A] = [C][P][C]$$

Thus equation (10) becomes

$$[C][P][C][U] = \lambda[C]^2[U]$$

$$[C][P][X] = \lambda[C][X]$$

$$[P][X] = \lambda[X]$$

Where we have substituted $[C][U] = [X]$. $[X]$ is a $(n+1) \times 1$ dimensional matrix and $\lambda = \omega^2$. The problem is thus reduced to an Eigen value problem. This problem can be solved in the following manner

- Construct matrix $[B]$ and $[A]$ for given wave vector k.
- Construct matrix $[C]$ as given by equation (11).
- Construct matrix $[P]$ as given by equation (12).
- Find ω^2 as the Eigen values of $[P]$. There will be $(n+1)$ values of ω^2 for given k.
- Repeat the above steps for different values of k and plot the dispersion relation.

2.3 Matlab programs:

Matlab programming has been used to simulate the problem discussed in the above section. Following is the list of variables used in these programs-

c4a = Elastic constant c44 for Aluminum Nitride

c4g = Elastic constant c44 for Gallium Nitride

c6a = Elastic constant c66 for Aluminum Nitride

c6g = Elastic constant c66 for Gallium Nitride

c44 = Elastic constant c44 for Gallium Nitride

c66 = Elastic constant c66 for Gallium Nitride

rg = Density of Gallium Nitride

ra = Density of Aluminum Nitride

tg = Thickness of Gallium Nitride

ta = Thickness of Aluminum Nitride

k = wave vector

kz = z component of wave vector

w = angular frequency

vt = Transverse acoustic wave velocity in bulk GaN.

For evaluating the phonon group velocity first order Newton finite difference has been used.

2.3.1 Program for phonon dispersion relation in free standing nanostructure:

```
% this script plot the angular frequency w vs wave vector k
% for each quantized value of kz, w is evaluated over linear space
% k which has 200 elements. Each curve in the plot correspond to a value
% of kz. Thickness of GaN slab is 6nm and there are 6 phonon branches.
% Thus ‘i’ is varying from 1 to 6.
close all
clear all
clc
 c44=10.5*10^11;
c66=12.3*10^11;
rg=6.15;
k=(linspace(10^7,10^8,200))';
kz=[ ];w=[ ];z=[ ];

for i=1:6
   kz=[kz;i*pi/(6*10^-7)];
    w=[w,sqrt((c66*k.^2+c44*kz(i)^2)/rg)];
end

plot(k,w)
xlabel('k');
ylabel('w');
hold on
plot(k,k*sqrt(c66/rg),'k:')
hold off
```

2.3.2 Program for phonon dispersion relation in heterostructure

```
%   This script is used to plot the phonon dispersion relation for
%   AlN/GaN/AlN Heterostructure. N+1 corresponds to number
```

```
%  of branches.


close all
clear all
clc
n = input('enter the value of n ');
g = input('enter the core thickness');
a = input('enter the cladding thickness');
c4a = 12.5*10^11;
c4g = 10.5*10^11;
c6a = 11.2*10^11;
c6g = 12.3*10^11;
rg = 6.15;
ra = 3.255;
tg = g*10^(-7);
ta = a*10^(-7);
z0 = - (tg+2*ta)/2;
h = (tg+2*ta)/n;
z=[ ];rho=[ ]; c44=[ ]; c66=[ ]; af=[ ];
for i=0:n
   z=[z,z0+i*h];
end
for i=1:n+1
   if (-tg/2<=z(i))&&(z(i)<tg/2)
      rho=[rho,rg];
      c44=[c44,c4g];
      c66=[c66,c6g];
   else
      rho=[rho,ra];
      c44=[c44,c4a];
      c66=[c66,c6a];
   end
```

```
end
l=0;
for j=0:0.001:5
   l=l+1;
   k(l)=j*10^(7);
   %constucting matrix A
   a=zeros(n+1);
   a(1,1)=-2*c4a/h^2-c6a*k(l)^2;
   a(n+1,n+1)=-2*c4a/h^2-c6a*k(l)^2;
   a(1,2)=2*c4a/h^2;
   a(n+1,n)=2*c4a/h^2;
   for i=2:n
      a(i,i-1)=(-c44(i+1)+4*c44(i)+c44(i-1))/(4*h^2);
      a(i,i)=-2*c44(i)/h^2-c66(i)*k(l)^2;
      a(i,i+1)=(c44(i+1)+4*c44(i)-c44(i-1))/(4*h^2);
   end
   b=-diag(rho);
   c=sqrt(b);
   p=c^(-1)*a*c^(-1);
   wsqr=eig(p);
   w=sqrt(wsqr);
   af=[af,w];
end
plot(k,af','.','markersize',0.5);
xlabel('k value');
ylabel('Angular frequency');
```

2.3.3 Program for group velocities in free standing nanostructure

```
% this script plot the angular frequency w vs wave vector k
% for each quantized value of kz w is evaluated over linear space
```

```
% k which has 200 elements. Each curve in the plot correspond to a value
% of kz. our GaN slab is 6nm and there are 6 phonon branches. Thus i is
% varying from 1 to 6. Newton first order difference has been used for the
% differentiation.
clc
clear;
c44=10.5*10^11;
c66=12.3*10^11;
rg=6.15;
vt=sqrt(c66/rg);
k=(linspace(0,0.5*10^8,200))';
kz=[];w=[];z=[];
for i=1:6
   kz=[kz;i*pi/(6*10^-7)];

   w=[w,sqrt((c66*k.^2+c44*kz(i)^2)/rg)];
end
h=k(2)-k(1);
w1=w(:,1);
w2=w(:,2);
w3=w(:,3);
w4=w(:,4);
w5=w(:,5);
w6=w(:,6);
d1=[0;diff(w1)]./h;
d2=[0;diff(w2)]./h;
d3=[0;diff(w3)]./h;
d4=[0;diff(w4)]./h;
d5=[0;diff(w5)]./h;
d6=[0;diff(w6)]./h;
plot(k,d1,k,d2,k,d3,k,d4,k,d5,k,d6)
hold on;
```

```
b = linspace(vt, vt, 200);
plot(k,b,'k-')
axis([0 5*10^7 0 5*10^5])
xlabel('wave vector k cm^-1');
ylabel('group velocity v cm/s');
title('group velocity for 6nm free standing nanostructure')
```

2.3.4 Program for group velocities in heterostructure with varying thickness

```
% This script plot the group velocity against wave vector in heterostructure.
% The script is only valid for total thickness of 6nm.
clc
close all
clear;
n=5;
g=input('enter the core thickness');
a=input('enter the cladding thickness');
c4a=12.5*10^11;
c4g=10.5*10^11;
c6a=11.2*10^11;
c6g=12.3*10^11;
rg=6.15;
ra=3.266;
vt=sqrt(c6g/rg);
tg=g*10^(-7);
ta=a*10^(-7);
z0=-(tg+2*ta)/2;
h=(tg+2*ta)/n;
z=[];rho=[];c44=[];c66=[];af=[];km=[];afm1=[];afm2=[];afm3=[];
afm4=[];afm5=[];afm6=[];
for i=0:n
```

```
    z=[z,z0+i*h];
end
for i=1:n+1
    if (-tg/2<=z(i))&(z(i)<tg/2)
        rho=[rho,rg];
        c44=[c44,c4g];
        c66=[c66,c6g];
    else
        rho=[rho,ra];
        c44=[c44,c4a];
        c66=[c66,c6a];
    end
end
l=0;
for j=0:0.001:6
    l=l+1;
    k(l)=j*10^(7);
    %constucting matrix A
    a=zeros(n+1);
    a(1,1)=-2*c4a/h^2-c6a*k(l)^2;
    a(n+1,n+1)=-2*c4a/h^2-c6a*k(l)^2;
    a(1,2)=2*c4a/h^2;
    a(n+1,n)=2*c4a/h^2;
    for i=2:n
        a(i,i-1)=(-c44(i+1)+4*c44(i)+c44(i-1))/(4*h^2);
        a(i,i)=-2*c44(i)/h^2-c66(i)*k(l)^2;
        a(i,i+1)=(c44(i+1)+4*c44(i)-c44(i-1))/(4*h^2);
    end
    b=-diag(rho);
    c=sqrt(b);
    p=c^(-1)*a*c^(-1);
    wsqr=eig(p);
```

```
    w=sqrt(wsqr);
     af=[af,w];
    afm1=[afm1,w(1)];
    afm2=[afm2,w(2)];
    afm3=[afm3,w(3)];
    afm4=[afm4,w(4)];
    afm5=[afm5,w(5)];
    afm6=[afm6,w(6)];
end
h=k(2)-k(1);
d1=[0,diff(afm1)./h];
d2=[0,diff(afm2)./h];
d3=[0,diff(afm3)./h];
d4=[0,diff(afm4)./h];
d5=[0,diff(afm5)./h];
d6=[0,diff(afm6)./h];
plot(k,d1,'.','markersize',0.5);
hold on;
plot(k,d2,'.','markersize',0.5);
plot(k,d3,'.','markersize',0.5);
plot(k,d4,'.','markersize',0.5);
plot(k,d5,'.','markersize',0.5);
plot(k,d6,'.','markersize',0.5);
hold on;
b = linspace(vt, vt, 6001);
plot(k,b,'k--','linewidth',1.5)
axis([0 5*10^7 0 6*10^5])
xlabel('Wave vector k cm^-1');
ylabel('Phonon group velocity cm/s');
title('Group velocity in AlN/GaN/AlN   2nm/2nm/2nm')
```

Chapter 3
Results and discussion

3.1 Input data for program

Matlab programs discussed in chapter 2 have some variables and needs to be input. These are basically elastic constants and mass density for gallium nitride and aluminum nitride. One more variable is 'n' that is the no of phonon branches possible in the given width of core. All the input to programs is described below:

Material constants [32] and mass density [33][34] of GaN and AlN used in the model.

C44 for Aluminum Nitride = 12.5*10^11 dyne cm^{-2}

C44 for Gallium Nitride = 10.5*10^11 dyne cm^{-2}

C66 for Aluminum Nitride = 11.2*10^11 dyne cm^{-2}

C66 for Gallium Nitride = 12.3*10^11 dyne cm^{-2}

Density of Aluminum Nitride = 3.255 gm cm^{-3}

Density of Gallium Nitride = 6.15 gm cm^{-3}

3.2 Number of phonon branches

There exists number of phonon branches. Their existence can be explained by the quantization of lattice waves along the z axis due to partial or complete phonon spatial confinement along the cross-plane direction. The total number of phonon branches can be found by the ratio t/2c, where 't' is the total thickness of the heterostructure or the single thin film and 'c' is the lattice constant of the material. For Wurtzite GaN the approximate value of lattice constant along c axis is 0.51 nm. Thus number of phonon branches possible in structure of width 6nm and 10nm are 6 and 10 respectively. The variable n the program when incremented by one, gives the number of phonon branches.

3.3.1 Phonon dispersion relation for the bulk and free standing nanostructure:

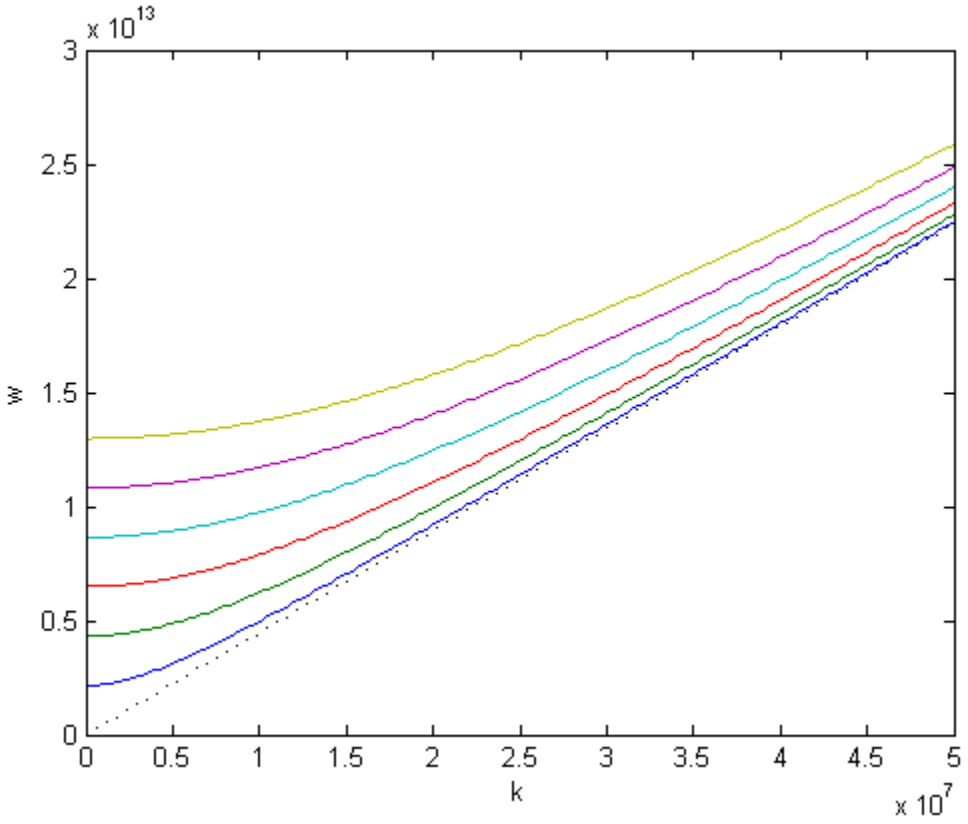

Figure 3.1: Solid lines showing the dispersion relation for free-surface single GaN thin film with a thickness of 6 nm. The dashed line shows the dispersion relation for the transverse acoustic waves in bulk GaN. Along x axis is the wave vector (k) and along y axis is the angular frequency (ω).

Fig. 3.1 shows the dispersion relation of free standing nano structure. The observations inferred from this figure are as follows.

1. The phonon dispersion in nano structure is different from that in bulk.
2. In nano structure, for given k a phonon can have set of discrete frequency values. This is due to the spatial confinement of phonons in z direction, which leads to quantization of k_z.
3. Change in slope signifies the change in group velocity of phonons and hence thermal properties.

4. The dashed line in figure represents the transverse acoustic phonon dispersion in bulk GaN, which is given by ω=k*sqrt(c66/ρ)

3.3.2 Group velocity plot for free standing nano structure:

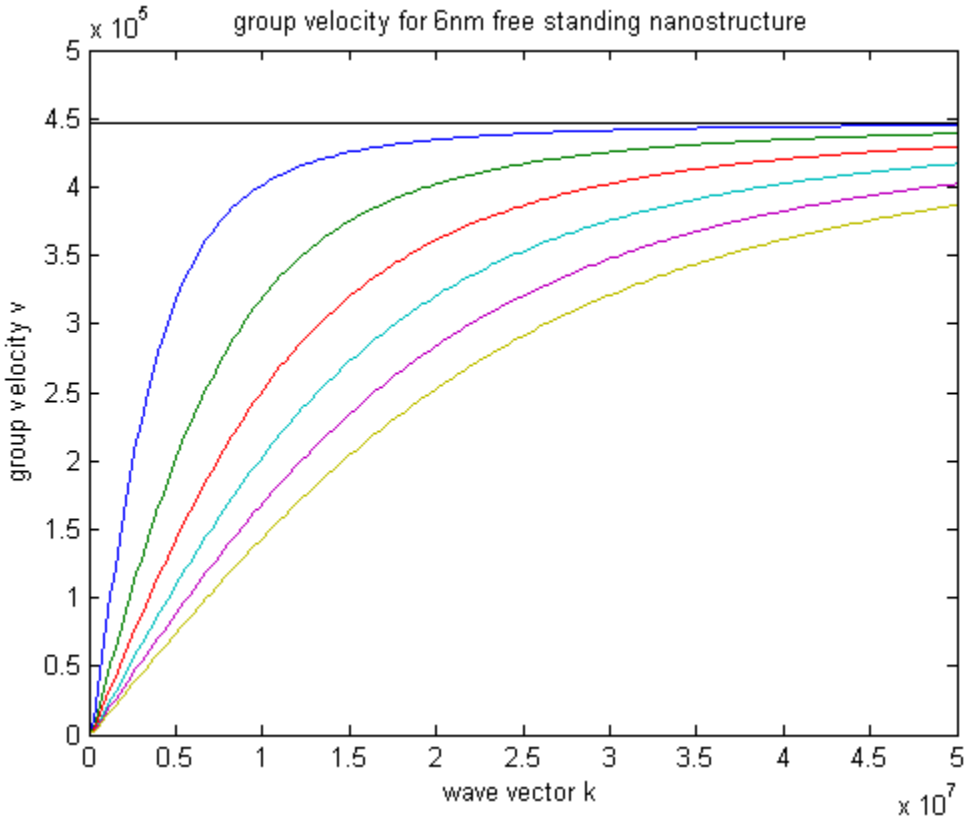

Figure 3.2: Group velocities for 6nm free standing nanostructure.

Fig. 3.2 shows the group velocities for free standing nano structure. The observations inferred from this figure are as follows.

1. Six curves show the group velocity corresponding to six phonon branches.
2. Straight line represents the phonon group velocity in bulk structure.
3. The group velocity has been reduced in the nanostructure due to complete phonon confinement.
4. Group velocity approaches to zero as wave vector approaches to zero.

3.3.3 **Phonon dispersion relation for the heterostructure with varying thickness:**

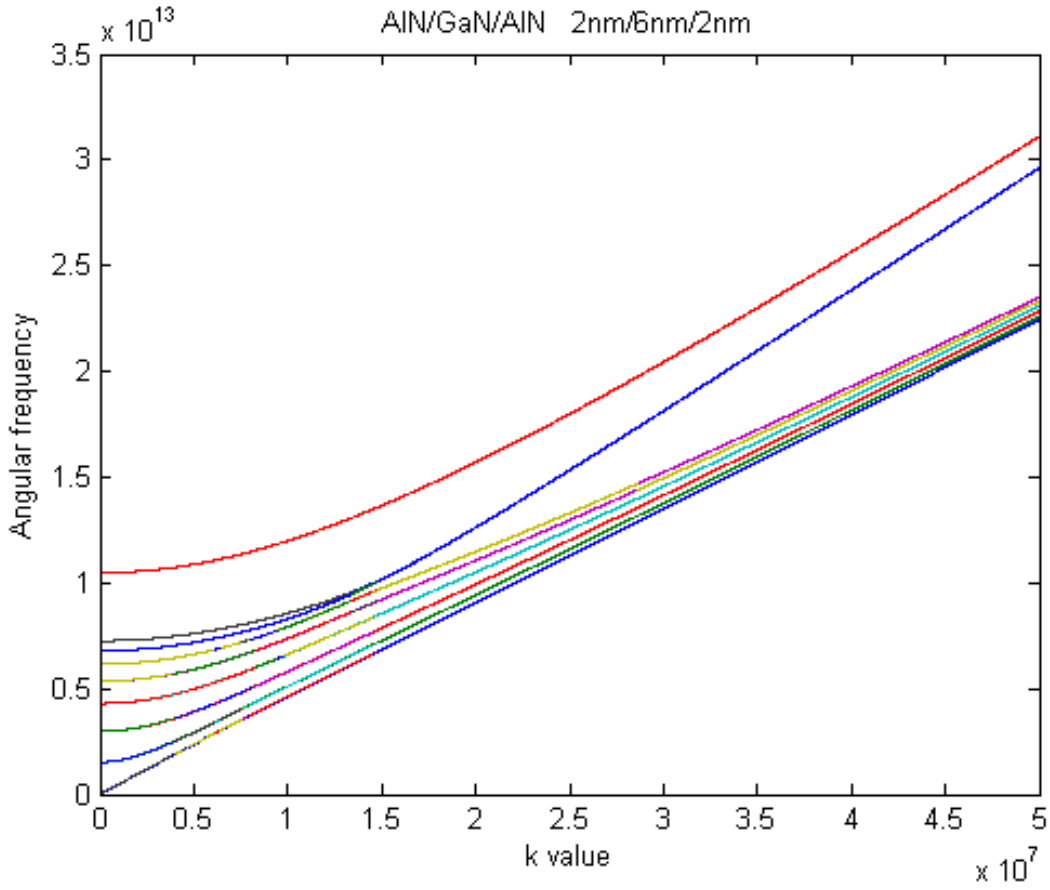

Figure 3.3.1: Phonon dispersion in AlN/GaN/AlN heterostructure with layer widths as 2nm/6nm/2nm. There are total 10 phonon branches.

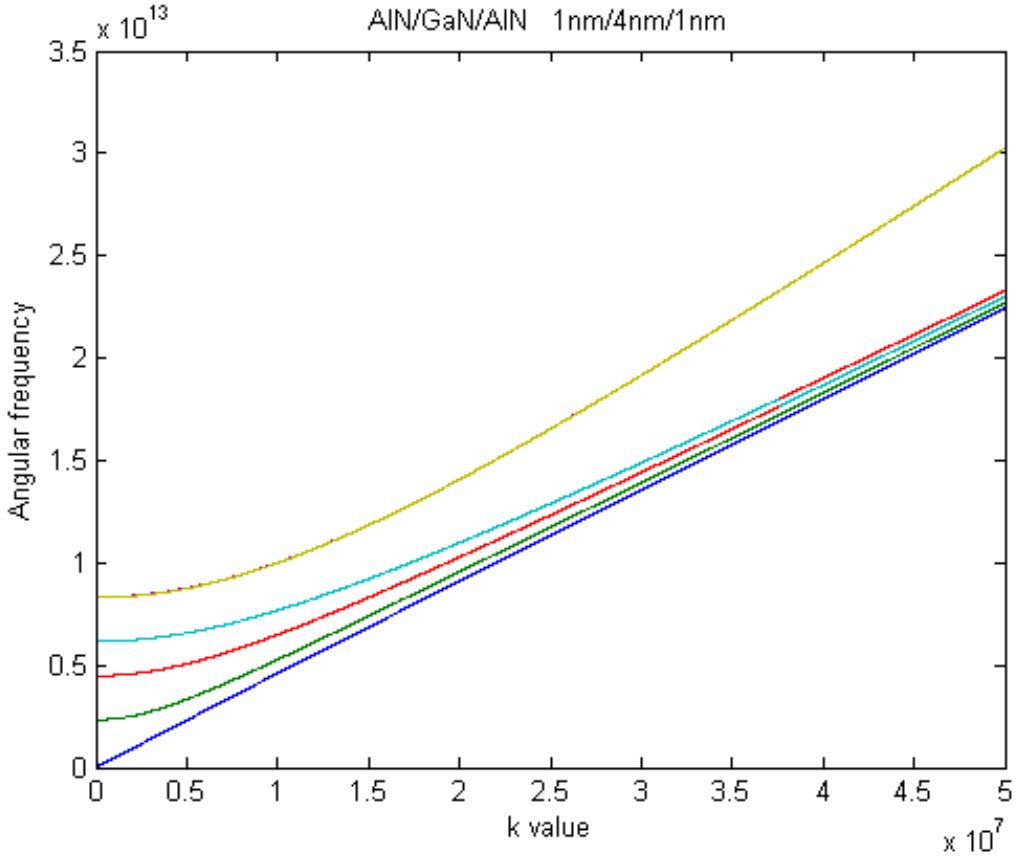

Figure 3.3.2: Phonon dispersion in AlN/GaN/AlN heterostructure with layer widths as 1nm/4nm/1nm. There are total 6 phonon branches. The above two branches are merging with each other

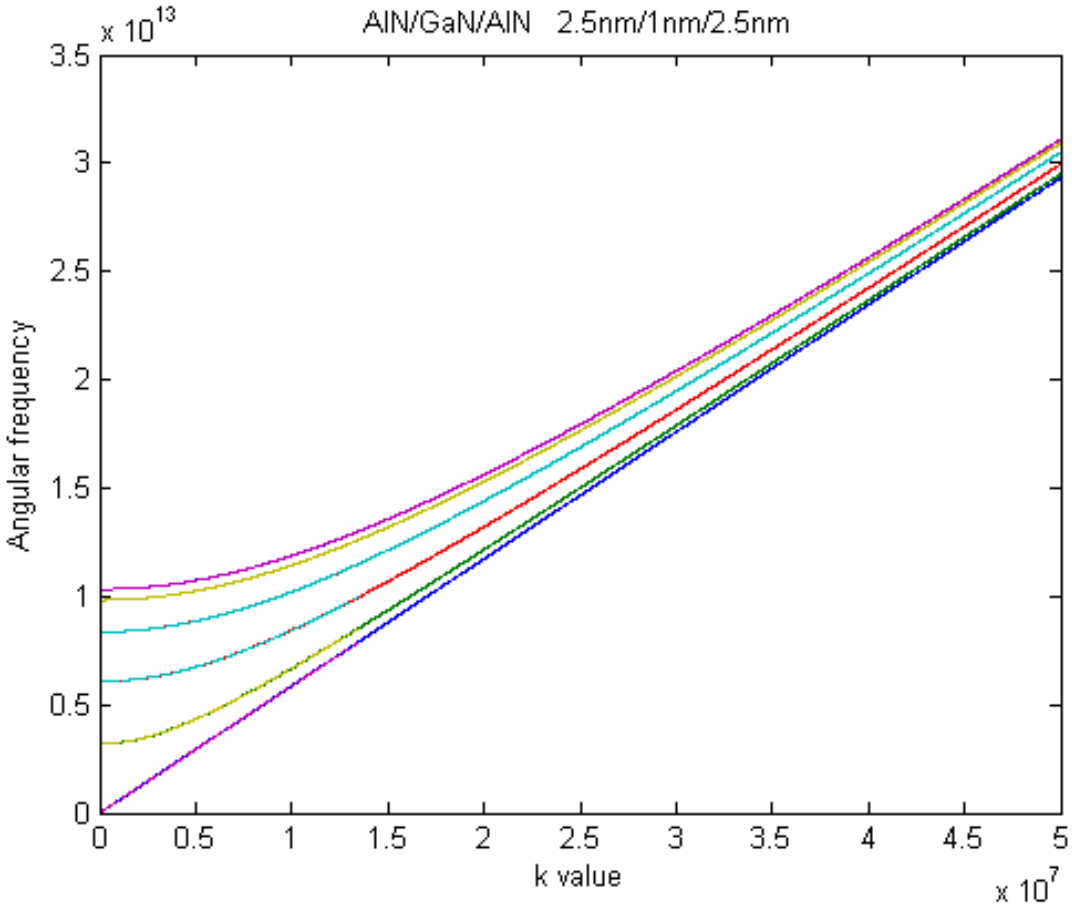

Figure 3.3.3: Phonon dispersion in AlN/GaN/AlN heterostructure with layer widths as 2.5nm/1nm/2.5nm. There are total 6 phonon branches.

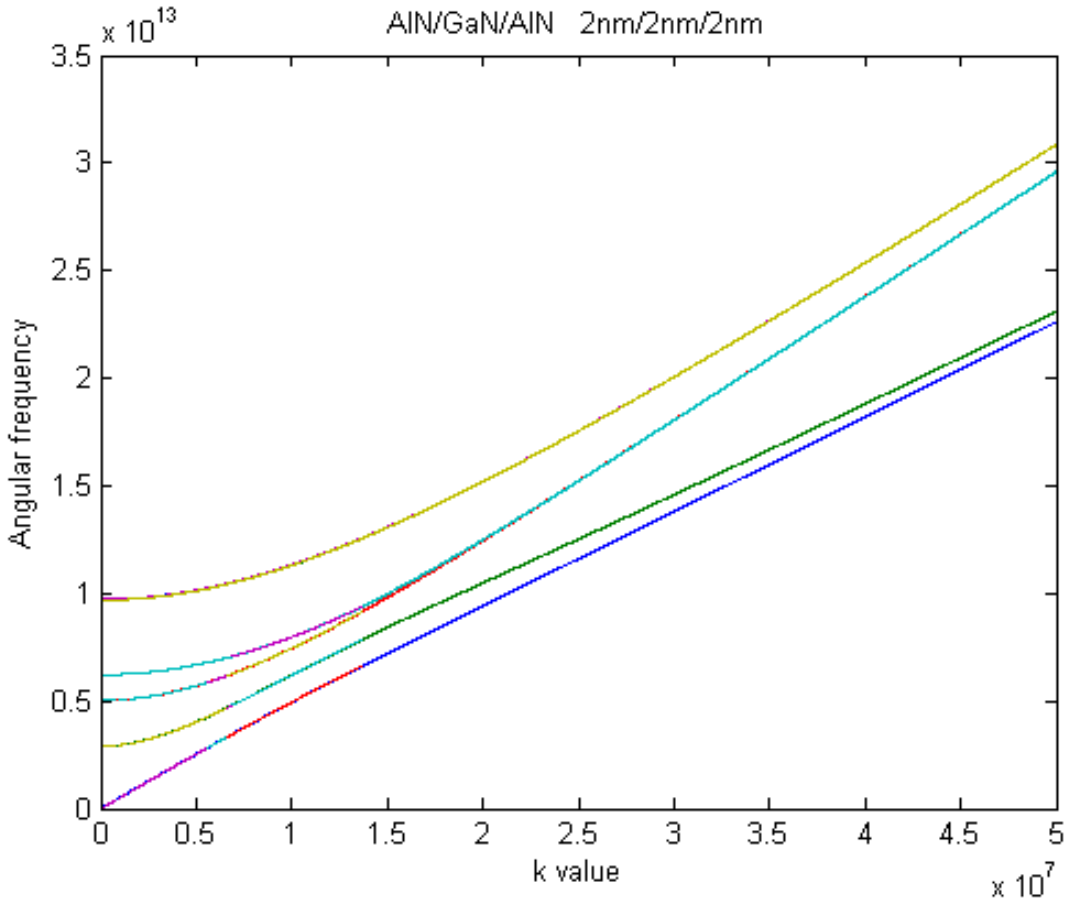

Figure 3.3.4: Phonon dispersion in AlN/GaN/AlN heterostructure with layer widths as 2nm/2nm/2nm. There are total 6 phonon branches. The above two branches are merged together.

Above figures (3.3.1 – 3.3.4) shows the dispersion relation of GaN/AlN/AlN heterostructure. The observations inferred from this figure are as follows.

1. Phonon dispersion is modified due to partial phonon confinement.
2. Cut-off frequency for each phonon branch in the heterostructure has been reduced as compared to free standing nanostructure.
3. The slope of lines has been changed, which signifies the change of phonon group velocity.
4. Phonon energy (ω multiplied by ħ) for given branch has been decreased as compared to free standing GaN nanostructure. The reason behind this is that the lattice waves in the GaN core layer penetrates into the AlN cladding layers due to partial phonon spatial confinement. This spreading of the lattice waves increases the phonon wavelength in the GaN core region and consequently decreases the phonon energy

3.3.4 Group velocity in heterostructure with varying thickness:

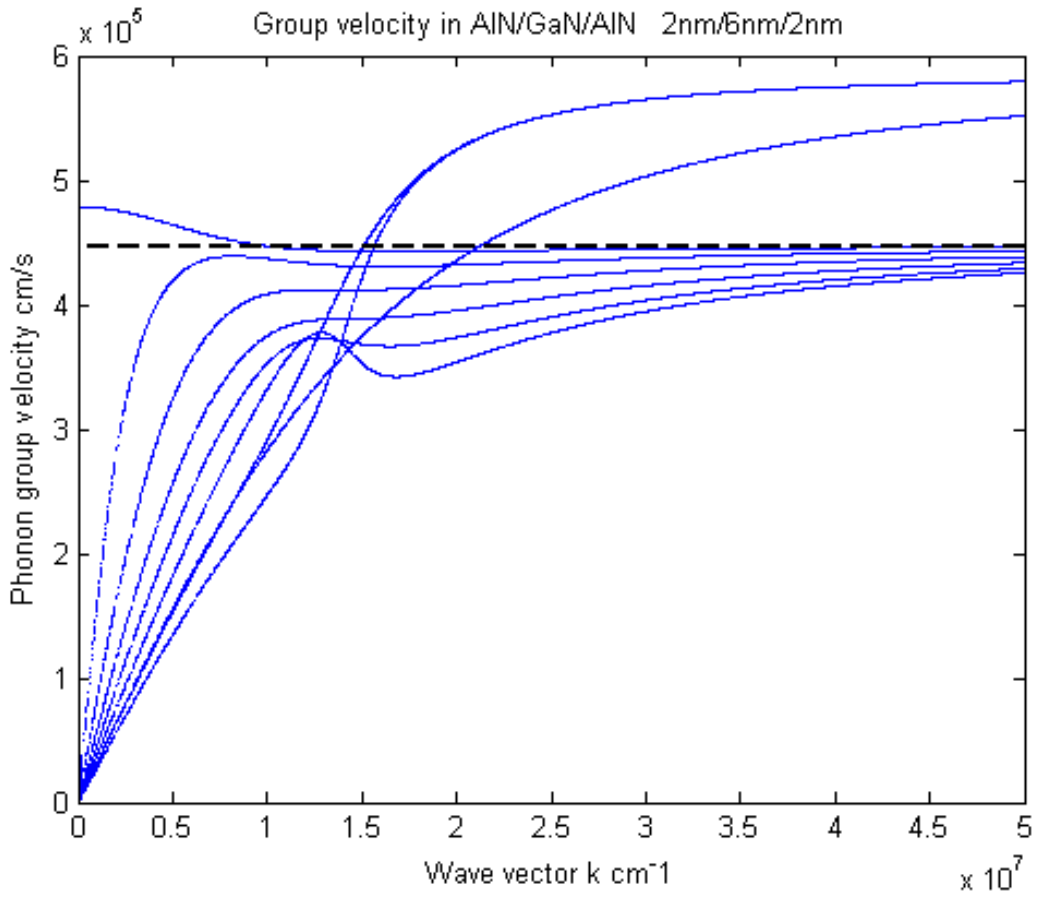

Figure 3.4.1: Group velocities in AlN/GaN/AlN heterostructure with layer widths 2nm/6nm/2nm. The dotted line represents the bulk velocity for GaN.

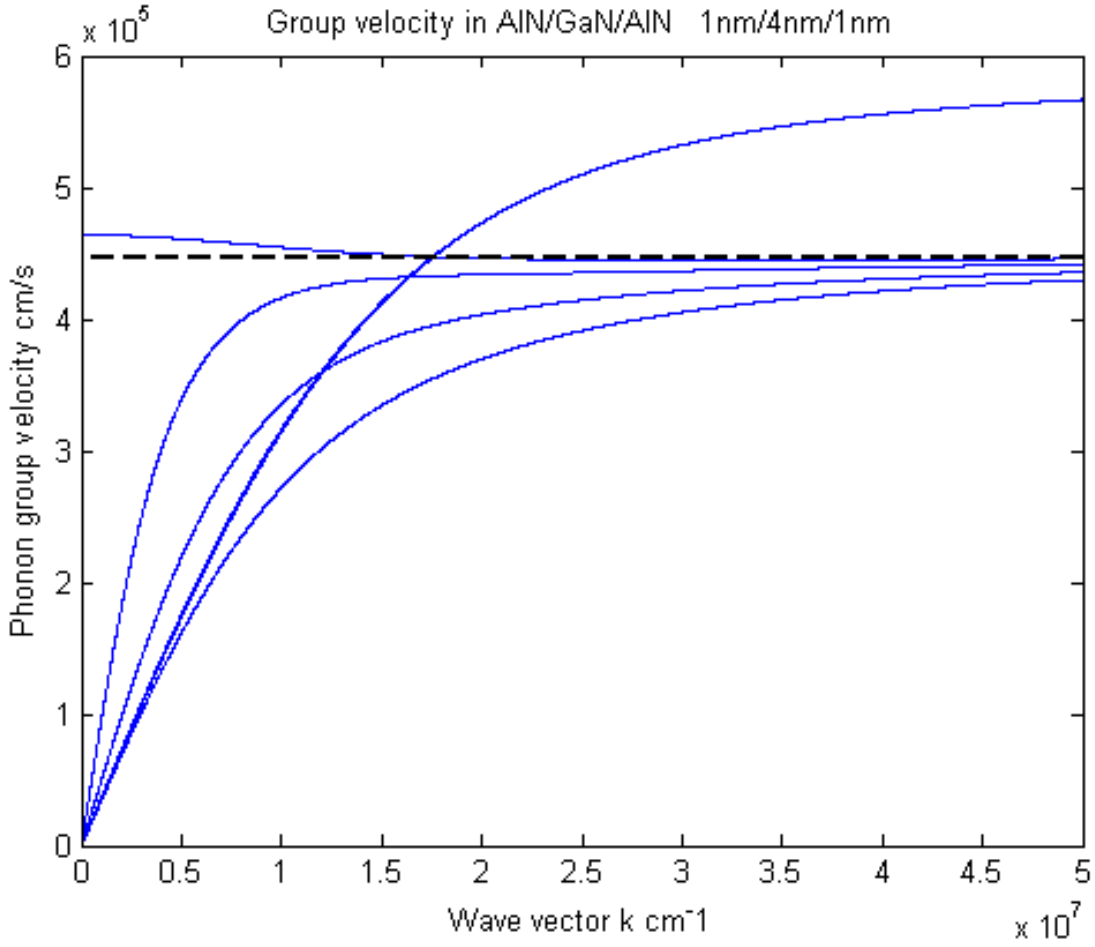

Figure 3.4.2: Group velocities in AlN/GaN/AlN heterostructure with layer widths 1nm/4nm/1nm. The dotted line represents the bulk velocity for GaN.

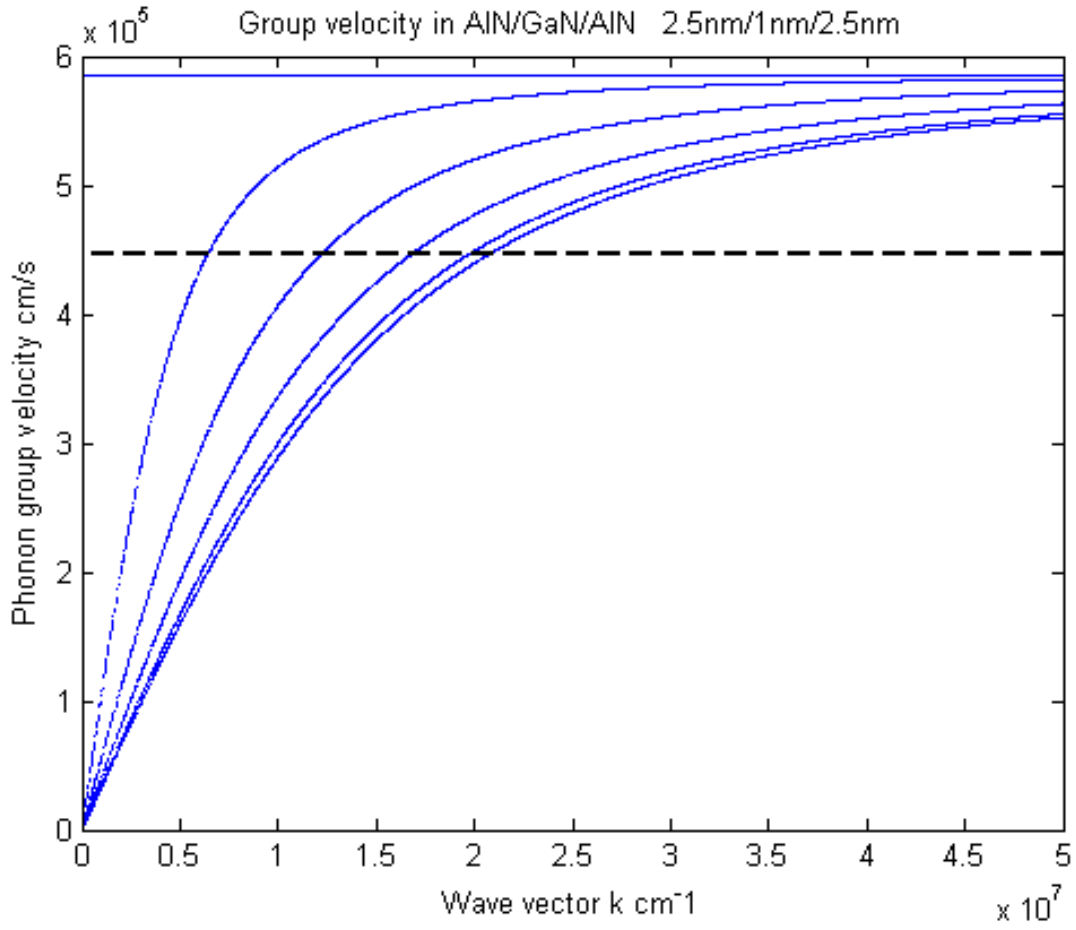

Figure 3.4.3: Group velocities in AlN/GaN/AlN heterostructure with layer widths 2.5nm/1nm/2.5nm. The dotted line represents the bulk velocity for GaN.

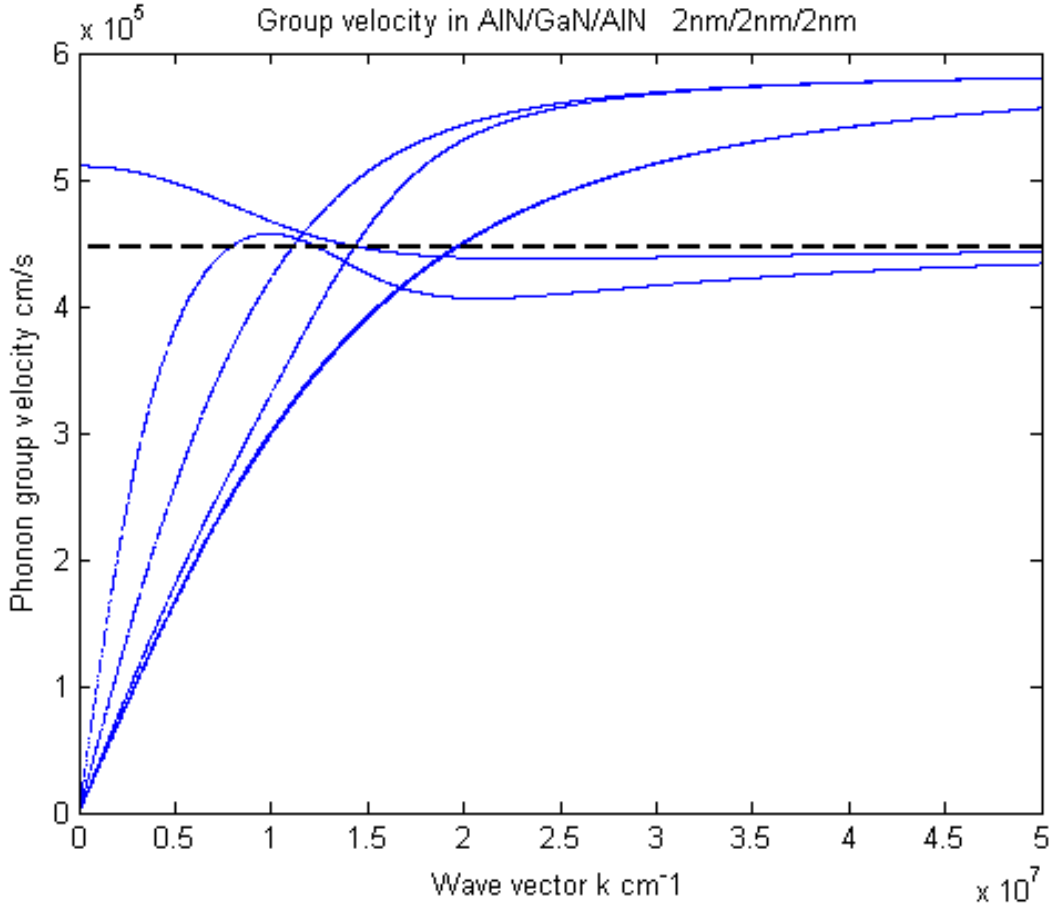

Figure 3.4.4: Group velocities in AlN/GaN/AlN heterostructure with layer widths 2nm/2nm/2nm. The dotted line represents the bulk velocity for GaN.

Above figures (3.4.1 – 3.4.4) shows the group velocities for AlN/GaN/AlN heterostructure with varying thickness. The observations inferred from this figure are as follows.

1. Horizontal dotted line represents the phonon group velocity in the bulk.
2. Some phonon branches have more group velocity as compared to bulk.
3. As the core thickness is decreased more and more phonon branches have group velocity greater than the bulk. For core thickness equal to 1nm all the phonon branches are having group velocity greater than bulk.
4. No phonon branch has velocity more than that in bulk cladding material. Here cladding is of Aluminum Nitride with sound velocity = $5.856*10^5$ cm/s.

3.4 Discussion:

The phonon dispersion relations for free standing GaN nanostructure and AlN/GaN/AlN heterostructure has been plotted and utilized to study the phonon group velocities in these structures. The affect of phonon confinement on the two structures is different. Group velocity is suppressed in one case and enhanced in the other.

Figure 3.1 shows that the variation of ω with k is linear for bulk (shown by dotted line). On the other hand in free standing GaN nanostructure variation of w with k is anomalous which has also been shown in the same figure (curved lines). This figure also shows the existence of multiple phonon branches in case of free standing GaN heterostructure. Figure 3.2 shows the variation of group velocity (dω/dk) with wave vector k for both the bulk material and free standing GaN nanostructure. There is considerable decrease in group velocity from its bulk value. The group velocity for bulk GaN is represented by a straight line. The reduced group velocity will result in reduced thermal conductivity. This result has also been corroborated by D. Li *et al*. it is experimentally observed that the thermal conductivity of Si nanowires can be two orders lower than its bulk value [35].

In case of AlN/GaN/AlN heterostructure an anomalous dispersion similar to free standing GaN nanostructure has been observed. There are two basic differences between the phonon dispersion plots for the free standing GaN nanostructure and AlN/GaN/AlN heterostructure. Firstly, some phonon branches exhibits relatively more slopes. Secondly, the cut-off frequency is lowered for each branch. Such difference exists due to different types of phonon confinement in these two structures. In case of free standing GaN nanostructure phonon bears complete confinement whereas in heterostructure there is partial phonon confinement.

Phonon dispersion for AlN/GaN/AlN heterostructures with varying core and cladding thickness has been obtained in section 3.3.4. Strong effect on the dispersion curves is observed. As the core thickness is decreasing more and more branches are having larger slope as compared to free standing GaN nanostructure. In figures 3.3.2 - 3.3.4 the total thickness of the heterostructures is kept constant and hence there are same numbers of phonon branches.

In section 3.3.4 variation of group velocity with wave vector has been studied. Figure 3.4.1 shows the effect of embedding the GaN nanostructure into AlN cladding in contrast to

figure 3.2. Group velocity for some branches has been increased not only from there free standing value, but also from their bulk value. In figure 3.4.2 to 3.4.4 core thickness is varying but total thickness of the heterostructure is kept constant. As core thickness is decreasing more and more phonon branches are having group velocity greater than that of bulk GaN. For core thickness of 1nm all the phonon branches have group velocity more than their bulk value. The uppermost branch is travelling with velocity, which is approximately equal to bulk value of sound velocity for cladding material i.e. Aluminum Nitride. It has also been noticed that the uppermost limit of group velocity in core is decided by the bulk sound velocity for the cladding material. So apart from thickness, choosing the proper cladding material may be helpful in controlling the behavior of phonons, which in turns controls the physical properties required for device fabrication.

Chapter 4

Summary and Future Scope

4.1 Summary

AlN/GaN/AlN heterostructure is very important from device point of view. In general flow of electrons is impeded by the presence of phonons. More particularly heating of the interfaces would also be avoided in the application of the heterostructure for the devices. The dispersion of phonon is helpful in understanding the heat evolution and transmission in heterostructures.

The results presented in this thesis are related with the study of dispersion relation in the AlN/GaN/AlN heterostructure. Base of the study is related with numerical reduction of problem by using finite difference method. The programming of reduced problem has been done by using MATLAB. The following important conclusions have been drawn from the observed results.

1. Phonons show anomalous dispersion in free standing GaN nanostructure and AlN/GaN/AlN heterostructure in contrast to linear dispersion in bulk GaN sample.
2. Decrement in phonon group velocity for free standing GaN nanostructure from its bulk value.
3. Decrement in cut-off frequency for AlN/GaN/AlN heterostructure as compared to free standing GaN nanostructure.
4. Increment in Phonon group velocity for AlN/GaN/AlN heterostructure from its bulk value.
5. Enhancement in the phonon group velocity with decreasing core thickness. The upper limit to velocity is decided by the cladding material.
6. Proper choice of cladding material and core thickness could control the phonon group velocity which in turns in controls the heat dissipation in heterostructures.

Future Scope

Besides the studies presented in this thesis there are also some areas of technological and academic importance that needs further investigation. They are as follows.

1. The dispersion relation of AlN/GaN/AlN could also be explored at optical frequencies. This will be helpful in predicting the dielectric and optical behavior.
2. The dispersion relation of some other semiconductor heterostructure e.g. InSb/GaP/InSb need also to be explored.
3. The dispersion relation of nanomaterials such as nanotubes, nanowires, thin film and quantum dots need to be studied because it will be helpful in predicting the thermal behavior in low dimensional materials.

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