Lifetime Of Anharmonic Decay Of Optical Phonons In Confined GaAs Structure

BY

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THESIS

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LIST OF ABBREVIATIONS

F	Force
U_{2r} , U_{2r-1}, U_{2r+1}..	Displacement of atoms from corresponding equilibrium position
m, M	Mass of different atoms
Q	Wave vector
A	Is the normalization constant
ω	Frequency
T	Time
$\hbar\omega_q$	Energy is given by $\hbar\omega_q$
n_q	Number of phonons
K_B	The value of Boltzmann's **constant** is approximately 1.3807 x 10^{-23} joule s per kelvin (J. K^{-1})
T	Temperature
$a_q^\dagger$	Creation operator to represent the creation of phonons
a_q	Annihilation operator to represent that the phonon has been annihilated
u_q	Modes for computing amplitude of the phonon
u(r)	Phonon displacement, fourier series over the modes u_q

LIST OF ABBREVIATIONS (continued)

H_{Fr}	Frohlich Hamiltonian
N	Number of unit cells
μ	Electron mobility

SUMMARY

The expression for the lifetime of optical phonons in bulk material has been well researched; however, there aren't enough estimations for the theoretical lifetime of optical phonons in confined structures. In this research, the expression for lifetime of a confined optical phonon decaying in to two acoustical phonons in GaAs double heterointerface structures was derived.

For this scope of research, the anharmonic decay which is the three phonon decay process, where an optical phonon decays into two acoustic phonons is considered. The expression for the displacement of the optical phonons and acoustic phonons in three phonon decay process is used to estimate the Hamiltonian of the anharmonic decay. Using this Hamiltonian and the Fermi golden rule which gives the transition probability, the rate of transition and theoretical lifetime of phonon has been calculated.

We considered the sandwiched AlAs/GaAs/AlAs structure to study the optical phonons confined in GaAs. The estimation shows that the decay rate of phonon in confined GaAs structures has been reduced by half.

CHAPTER 1 INTRODUCTION

1.1 Motivation

Phonons and the interpretation of lattice dynamics are important to study the physical properties of crystals. These physical properties are studied in terms of phonon infrared scattering spectra, neutron scattering, Raman scattering, etc.

The following are some cases where the study of phonons and its lifetime are important. In semiconductors, the saturation velocity of the carriers depends upon the electron energy loss by LO phonon emission which measures the speed of a device. In a quantum well semiconductor laser, the electron must lose energy –which it can rapidly do by optical phonon emission events to be captured in the active region. Therefore, the switching time of such a device and of the quantum well laser depends on the decay rate of the emitted phonon since the optical phonon may reabsorb the emitted phonon until they decay into weakly coupling acoustic phonons. Also, the heat transport in a crystal is by the shorter wavelength phonons, which are of high frequency and transport the heat energy and help maintain a thermal equilibrium. The mean travel path of such phonons determines the heat energy transport. These are some cases where the relaxation time of phonon plays a significant role.

The lifetime of a decaying optical phonon explained by Cowley [10], estimates the strength of interaction of phonons and numerically summed it to determine the overall interaction strength.

Klemens [2] estimated the theoretical lifetime of decaying optical phonon into two acoustical phonons. He also estimates the interaction strength and rate of change of the occupation number using which he derives the lifetime. Klemens theory has the advantage that it can be modelled analytically while and Cowley's has greater precision. Nonetheless, there hasn't been significant work on the lifetime of anharmonic decay of optical phonon in confined GaAs structure.

In this research we have considered double interface hetero-structure. With advancements in the fields of semiconductors, where the device size has been shrunk to few nanometers, leading to a high density of semiconductor interfaces. Therefore, it is important to study about the phonons that are confined in these nanostructures.

1.2 Thesis Outline

The basic phonon properties and the various models to describe the phonons are explained in Chapter 2, with some emphasis on dispersion relations for optical and acoustic phonons. In Chapter 3, the anharmonic decay of phonons has been explained along with the Klemens channel and Ridley channel for the bulk material and the lifetime of bulk phonon has been studied. Chapter 4 brings out the prerequisites needed for lifetime of confined phonons like the interaction Hamiltonian, conservation of the anharmonic decay process, the displacement of optical and acoustic phonons in confined GaAs structure and the matrix element. Then the lifetime of the confined optical phonons in GaAs is derived. Chapter 5 is a brief conclusion on lifetimes of confined optical phonon with that of bulk phonons. In Chapter 6 the importance of

phonons in designing the current semiconductor devices has been explained based on industrial experience at Intel.

CHAPTER 2 PHONON PROPERTIES AND MODELS

2.1 What is a Phonon?

The crystals have periodic arrangement of atoms across its lattice. There are various kinds of forces acting between the atoms of a crystal, ideally at equilibrium these forces cancel out each other. However, in non-ideal case, considering the lattice to be an elastic arrangement of atoms, excitation of an atom causes a collective excitation. The quantum description of this collective excitation is called phonon. Compared to a photon which is a quantum of electromagnetic oscillation, the phonon is quantized lattice vibration. The phonon can be called as the "quantum of the lattice vibrations" and the energy of the phonon is $\hbar\omega$ where ω is the angular frequency of the excitation. In simple description phonon is a normal mode of vibration or simply lattice vibrations. Phonons have properties of wave-particle duality of quantum mechanics. The atoms that vibrate out of phase with each other are called optical phonons and acoustic phonons are those which vibrate in same phase. The optical phonons are of higher frequency, and the acoustic phonons are of lower frequency but cover a larger range of frequencies. The longer wavelength acoustic phonons with lower frequency give rise to sounds. The smaller wavelength phonons which have higher frequencies, contribute to heat transport in the crystal.

The study of phonons has become increasingly important in the field of heat transport, solid state physics, quantum electronics, optoelectronics and superconductivity. Also, the phonon interactions have significant effect on thermal conductivity and electrical conductivity.

2.1.1 Dispersion Relation of optical and acoustic phonons in bulk structures

To understand more about phonons, it is important to know about the dispersion relation of phonons (Born and Huang, 1988, P55) [3]. Let us consider a one dimensional diatomic crystal, which would be like a linear chain of atoms as shown in figure [1]. In diatomic crystal, the two atoms of different masses are placed alternatively across the chain with uniform separation 'a'. There are various forces acting keeping each atom attracted to each other atom. In such a case, the displacement of one atom will disturb the position of its neighboring atom which has strong force acting between them. For simplicity let us consider only the adjacent neighboring atoms are coupled. The atoms coupled to each other have forces interacting between them, which is like that of a spring with spring constant 'k' connecting the two atoms. This is described by Hooke's law, where the system can be considered to that of a harmonic oscillator.

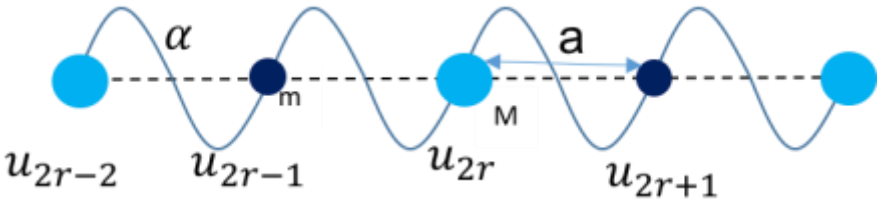

Figure 1: Linear chain model of atoms

The Hooke's law states that F=-ks, where k is the spring constant, F is the force, and s is the displacement [24]. In case of the phonons force is given by mass times acceleration. The displacement of two types of atom is given by equation 1 and 2.

$$u_{2r} = A_1 e^{i(2rqa-\omega t)} \quad (1)$$

and

$$u_{2r+1} = A_2 e^{i[(2r+1)qa-\omega t]} \quad (2)$$

where ω is the frequency and q is the phonon wave vector. Considering the mass m and M and substituting equation 1 and 2 in Hooke's law we get equation 7 and 8

$$m(d^2u_{2r}/dt^2) = -\alpha(u_{2r} - u_{2r-1}) - \alpha(u_{2r} - u_{2r+1}) \quad (3)$$

$$= \alpha(u_{2r+1} + u_{2r-1} - 2u_{2r}) \quad (4)$$

and

$$M(d^2u_{2r}/dt^2) = -\alpha(u_{2r+1} - u_{2r}) - \alpha(u_{2r+1} - u_{2r+2}) \quad (5)$$

$$= \alpha(u_{2r+2} + u_{2r} - 2u_{2r+1}) \quad (6)$$

$$-m\omega^2 A_1 = \alpha A_2\left(e^{iqa} + e^{-iqa}\right) - 2\alpha A_1 \quad (7)$$

and

$$-M\omega^2 A_2 = \alpha A_1\left(e^{iqa} + e^{-iqa}\right) - 2\alpha A_2 \quad (8)$$

Simplifying the above equations, eliminating A1 and A2 we get the frequency as

$$\omega^2 = \alpha\left(\frac{1}{m} + \frac{1}{M}\right) \pm \alpha\left[\left(\frac{1}{m} + \frac{1}{M}\right)^2 - \frac{4sin^2qa}{mM}\right]^{1/2} \quad (9)$$

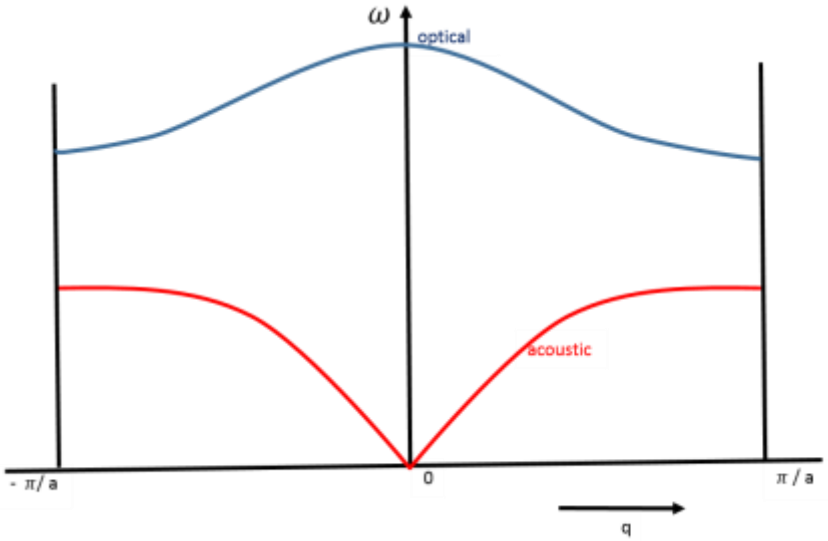

Figure 2: Dispersion Relation of phonons

In figure [2] it is shown that, the optical modes are of higher frequency but have short ranges of frequency whereas the acoustic phonons have lower frequencies but a wider range of frequencies.

The harmonic (Sakurai 1994) expression used here ignores the higher order terms of crystal potential (n>2) [8]. This approximation works well for the phonon dispersion curve. In our research as we deal with anharmonic decay we consider anharmonic or the higher order terms.

2.1.2 Phonon number, Creation and Annihilation Operator

The number of phonons at a given state having wave vector q is represented by nq. The phonon occupation number is given by

$$\hbar\omega_q(n_q + \tfrac{1}{2}) \tag{10}$$

it can also be rewritten as

$$n_q = \tfrac{1}{e^{\hbar\omega_q/k_BT} - 1} \tag{11}$$

The creation operator $a_q^\dagger$ increases the number of phonons n_q in a given state by one and the annihilation operator a_q decreases the number of phonons n_q by one.

$$a_q = \sqrt{\tfrac{m\omega_q}{2\hbar}u_q} - i\sqrt{\tfrac{1}{2\hbar m\omega_q}p_q} \tag{12}$$

and

$$a_q^\dagger = \sqrt{\tfrac{m\omega_q}{2\hbar}u_q} + i\sqrt{\tfrac{1}{2\hbar m\omega_q}p_q} \tag{13}$$

$$a_q^\dagger N_q \geq \left|\sqrt{n_q + 1}\right| N_q + 1\rangle \tag{14}$$

$$a_q|N_q \geq \sqrt{n_q}|N_q - 1\rangle \tag{15}$$

The change in phonon occupation number from an initial state to a final state represents the number of phonons decayed during the change of state.

2.1.3 Phonon Amplitude

The normal mode phonon displacement is given by

$$u_q = \sqrt{\frac{\hbar}{2m\omega_q}}(a_q + a_q^{\dagger}) \tag{16}$$

where $a_q \; and \; a_q^{\dagger}$ are the operators for creation and annihilation.

The amplitude of a phonon is represented by square of $\hbar/2\mathrm{m}\,\omega_q\,\mathrm{q}$ with the creation and annihilation operator which represents the number of phonons. From Stroscio and Dutta, 2001 we have

$$u(r) = \frac{1}{\sqrt{N}} \sum_q \sum_{j=1,2,3} \sqrt{\frac{\hbar}{2m\omega_q}} \, (a_q e^{iqr} \hat{e}_{q,j} + a_q^{\dagger} e^{iqr} \hat{e}_{q,j}) \tag{17}$$

where N is defined as the number of crystals unit cells [7]

2.1.4 Frohlich interaction

The relative displacement of negative and positive ions produces electric polarization p(r). The carrier phonon scattering occurs when charge carrier interacts with this polarization[2]. In GaAs, the carrier scattering at room temperature is by polar optical phonon scattering. This scattering is known as the Frohlich interaction. The potential energy due to this Frohlich interaction is denoted as $\Phi_{Fr}(r)$ and is given by

$$\nabla^2 \phi_{Fr}(r) = \; 4\pi e \nabla . P(r) \tag{18}$$

The above equation can be rewritten in terms of the creation operator and the annihilation operator as

$$P(r) = \; \zeta \sum_{j=1,2,3} \int \frac{d^3 q}{(2\pi)^3} (a_q e^{iq.r} e_{q,j} + a_q^{\dagger} e^{-iq.r} e_{q,j}^{*}) \tag{19}$$

where

$$4\pi\nabla.P(r) = \ 4\pi i\zeta \sum_{j=1,2,3} \int \frac{d^3q}{(2\pi)^3} (a_q e^{iq.r} e_{q,j} + a_q^{\dagger} e^{-iq.r} e_{q,j}^{*}) \tag{20}$$

the Frolich interaction Hamiltonian is given by the potential energy that is associated with the frolic interaction

$$H_{Fr} = \ \phi_{Fr}(r) = \ \int \frac{d^3q}{(2\pi)^3} (a_q e^{iq.r} - a_q^{\dagger} e^{-iq.r}) \tag{21}$$

the electric polarization P(r) may be written as

$$\mathrm{P(r)} = \frac{Ne^*}{\epsilon(\infty)} u_q(r) \tag{22}$$

$$u_q(r) = \ \frac{1}{\sqrt{N}} \sum_q \sum_{j=1,2,3} \sqrt{\frac{\hbar}{2\left(\frac{mM}{m+M}\right)\omega_{LO}}} \tag{23}$$

$$\zeta = \sqrt{\frac{\hbar}{2\omega_{LO}} \frac{\omega_{LO}^2}{4\pi} \left[\frac{1}{\epsilon(\infty)} - \ \frac{1}{\epsilon(0)}\right]} \tag{24}$$

and

$$H_{Fr} = \ -i\sqrt{\frac{2\pi e^2 \hbar\omega_{LO}}{V} \left[\frac{1}{\epsilon(\infty)} - \ \frac{1}{\epsilon(0)}\right]} \sum_q \frac{1}{q} (a_q e^{iq.r} - a_q^{\dagger} e^{-iq.r}) \tag{25}$$

2.1.5 Deformation potential

The lattice distortion gives rise to local changes in energy band which in turn represents the deformation potential interaction. One of the most important interaction in recent semiconductor devices is the deformation potential interaction. It was introduced by Bardeen and Shockley

(1950) [9]. It is dependent on the origin of the displacement which are caused by phonon interaction. The energy of the valence band or conduction band will change by an amount

$$E_v = E_v(a) - E_v(a+u)$$

$$E_c = E_c(a) - E_c(a+u) \quad (26)$$

where u is the displacement produced by the phonon mode and a is the lattice constant. Since a>>u it follows that

$$\Delta E_{c,v}(a) = (dE_{c,v}(a)/da)u \quad (27)$$

Deformation potential represents the important scattering in non-polar semiconductors. Most of the sources of electron energy loss in electronic devices made of semiconductor is due to deformation potential interaction. The energy is generalized as

$$\Delta E_{c,v}(a) = (dE_{c,v}(a)/dV)\Delta V \quad (28)$$

Where V is a volume element and AV is the change in the volume element. For an isotropic medium it becomes

$$\Delta E_{c,v}(a) = V\left(\frac{dE_{c,v}(a)}{dV}\right)\Delta.u \quad (29)$$

$$H_{def}^{c,v} = \Delta E_{c,v}(a) = E_l^{c,v}\Delta.u \quad (30)$$

2.1.6 Piezoelectric Interaction

The polar crystal lacking an inversion symmetry have piezoelectric interaction. There is a macroscopic polarization in piezoelectric crystals when electric field is applied. This macroscopic polarization is by the acoustic phonons. The piezo electric interaction in cubic crystal is given in rectangular coordinates using the piezoelectric coupling coefficient and strain tensors as

$$P=\left\{\frac{1}{2}e_{x4}\left(\frac{\partial w}{\partial y}+\frac{\partial v}{\partial z}\right),\ \frac{1}{2}e_{x4}\left(\frac{\partial u}{\partial z}+\frac{\partial w}{\partial x}\right),\ \frac{1}{2}e_{x4}\left(\frac{\partial u}{\partial y}+\frac{\partial v}{\partial x}\right)\right\} \quad (31)$$

2.2 Phonon Model

2.2.1Phonons Dielectric Continuum Model

In polar material the optical phonon is modeled in dielectric continuum model. As the name indicates it is associated with the polarization produced by the lattice vibration. The potential is given by P(r) (Kim and Stroscio,1990)

$$\nabla^2\Phi(r)=4\pi\nabla.P(r) \quad (32)$$

$$E(r)=-\nabla\Phi(r) \quad (33)$$

$$P(r)=\chi_n(\omega)E(r) \quad (34)$$

$$\chi_n(\omega)=[\epsilon_n(\omega)-1]/4\pi \quad (35)$$

Using the Lyddane sachs Teller relation we get,

$$\epsilon_n(\omega) = \epsilon_n(\infty)\frac{\omega^2-\omega_{LO,n}^2}{\omega^2-\omega_{TO,n}^2} \tag{36}$$

$$\epsilon_n(\omega) = \epsilon_n(\infty)\frac{\omega^2-\omega_{LO,n,a}^2}{\omega^2-\omega_{TO,n,a}^2}\frac{\omega^2-\omega_{LO,n,b}^2}{\omega^2-\omega_{TO,n,b}^2} \tag{37}$$

for a medium n where the displacement field is related to E(r) and P(r)

$$-\mu_n\omega^2 u_n(r) = -\mu_n\omega_{0n}^2 u_n(r) + e_n^* E_{local}(r) \tag{38}$$

$$P(r) = n_n e_n^* u(n)_r + n_n\alpha_n E_{local}(r) \tag{39}$$

n_n is the number of unit cells in region n.

$\mu_n = \frac{m_n M_n}{m_n+M_n}$ is the reduced mass.

α_n is the electronic polarizability per unit cell.

by Lorentz relation,

$$E_{local}(r) = E(r) + \frac{4\pi}{3}P(r) \tag{40}$$

for a ternary medium AC(BC) we have,

$$-\mu_{m,a(b)}\omega^2 u_{m,a(b)}(r) = -\mu_n\omega_{0m,a(b)}^2 u_{m,a(b)}(r) + e_{m,a(b)}^* E_{local}(r) \tag{41}$$

$$P(r) = n_m\left[y e_{m,a}^* u_{m,a}(r) + (1-y)e_{m,b}^* u_{m,b}(r)\right] + n_m\alpha_n E_{local}(r) \tag{42}$$

For a diatomic polar material we get

$$\ddot{u} = -\omega_{TO}^2 u + \left(\frac{V}{4\pi\mu N}\right)^{\frac{1}{2}}\sqrt{\epsilon(0)-\epsilon(\infty)}\;\omega_{TO}E \tag{43}$$

$$P = \left(\frac{\mu N}{4\pi V}\right)^{1/2}\sqrt{\epsilon(0)-\epsilon(\infty)}\;\omega_{TO}u + \left[\frac{\epsilon(\infty)-1}{4\pi}\right]E \tag{44}$$

For the Uniaxial wurzite structures we have

$$\ddot{u}_{\perp,n} = -\omega_{TO,\perp,n}^2 u_{\perp,n} + \sqrt{\frac{V}{4\pi\mu_n N}}\sqrt{\epsilon(0)_{\perp,n} - \epsilon(\infty)_{\perp,n}}\omega_{TO,\perp,n} E_{\perp,n} \tag{45}$$

$$P_{\perp,n} = \left(\frac{\mu_n N}{4\pi V}\right)^{1/2}\sqrt{\epsilon(0)_{\perp,n} - \epsilon(\infty)_{\perp,n}}\omega_{TO,\perp,n} u_{\perp,n} + \left[\frac{\epsilon(\infty)_{\perp,n}-1}{4\pi}\right]E_{\perp,n} \tag{46}$$

$$\epsilon_{\perp,n}(\omega) = \epsilon_{\perp,n}(\infty)\left(\frac{\omega^2-\omega_{LO,\perp,n}^2}{\omega^2-\omega_{TO,\perp,n}^2}\right) \tag{47}$$

$$\ddot{u}_{\parallel,n} = -\omega_{TO,\parallel,n}^2 u_{\parallel,n} + \sqrt{\frac{V}{4\pi\mu_n N}}\sqrt{\epsilon(0)_{\parallel,n} - \epsilon(\infty)_{\parallel,n}}\omega_{TO,\parallel,n} E_{\parallel,n} \tag{48}$$

$$P_{\parallel,n} = \left(\frac{\mu_n N}{4\pi V}\right)^{1/2}\sqrt{\epsilon(0)_{\parallel,n} - \epsilon(\infty)_{\parallel,n}}\omega_{TO,\parallel,n} u_{\parallel,n} + \left[\frac{\epsilon(\infty)_{\parallel,n}-1}{4\pi}\right]E_{\parallel,n} \tag{49}$$

$$\epsilon_{\parallel,n}(\omega) = \epsilon_{\parallel,n}(\infty)\left(\frac{\omega^2-\omega_{LO,\parallel,n}^2}{\omega^2-\omega_{TO,\parallel,n}^2}\right) \tag{50}$$

For the case of no free charge, these equations must be supported by the following electrostatics equation

$$E(r) = -\nabla\phi(r) \tag{51}$$

$$D(r) = E(r) + 4\pi P(r) \tag{52}$$

$$= \epsilon_{\perp}(\omega)E_{\perp}(r)\hat{\rho} + \epsilon_{\parallel}(\omega)E_{\parallel}(r)\hat{z} \tag{53}$$

$$\nabla.\mathrm{D(r)} = 0 \tag{54}$$

The above equation describes the carrier optical scattering in wurzite crystals

The perpendicular(parallel) displacement to the c axis is given by

$$u(r)_{\perp(\parallel)} = \frac{1}{\sqrt{N}}\sum_q \sum_{j=1,2,3}\sqrt{\frac{\hbar}{2m\omega_q}}\hat{e}_{q,j,\perp(\parallel)}\left(a_q + a_{-q}^{\dagger}\right)e^{iqr} \tag{55}$$

$$\phi(r)_{\perp(\parallel)} = \sum_q \phi(q)_{\perp(\parallel)}e^{iqr} \tag{56}$$

$$E(r)_{\perp(\parallel)} = -\nabla\phi(r)_{\perp(\parallel)} = iq\sum_q \phi(q)_{\perp(\parallel)}\, e^{iqr} \tag{57}$$

$$(\omega_{TO,\perp(\parallel)}^2 - \omega_q^2)\sqrt{\frac{\hbar}{2\mu_n N\omega_q}}\,\hat{e}_{q,j,\perp(\parallel)}(a_q + a_{-q}^\dagger) \tag{58}$$

$$= \sqrt{\frac{V}{4\pi\mu_n N}}\sqrt{\epsilon(0)_{\perp(\parallel),n} - \epsilon(\infty)_{\perp(\parallel),n}}\,\omega_{TO,\perp(\parallel),n}(-i)q_{\perp(\parallel)}\phi(q) \tag{59}$$

$$\sqrt{\frac{2\pi\hbar}{V\omega_q}}\,\hat{e}_{q,j,(\parallel)}\left(a_q + a_{-q}^\dagger\right) = \frac{\sqrt{\epsilon(0)_{\perp(\parallel),n} - \epsilon(\infty)_{\perp(\parallel),n}}\,\omega_{TO,\perp(\parallel),n}}{\omega_{TO,\perp(\parallel),n}^2 - \omega_q^2}(-i)q_{\perp(\parallel)}\phi(q) \tag{60}$$

For the isotropic case[] , the Lynddane-Sachs-Teller relation states that

$$\sqrt{\frac{2\pi\hbar}{V\omega_q}}\left(a_q + a_{-q}^\dagger\right)^2 = -q^2\left\{\frac{|\epsilon(0)_\perp - \epsilon(\infty)_\perp|\omega_{TO,\perp}^2}{(\omega_{TO_\perp}^2 - \omega_q^2)^2}sin^2\theta\right\}\phi^2(q) \tag{61}$$

$$= -q^2\left\{\frac{|\epsilon(0)_\parallel - \epsilon(\infty)_\parallel|\omega_{TO,\parallel}^2}{(\omega_{TO_\parallel}^2 - \omega_q^2)^2}cos^2\theta\right\}\phi^2(q) \tag{62}$$

$$\phi(q) = i\sqrt{\frac{2\pi\hbar}{Vq^2\omega_q}\left(a_q + a_{-q}^\dagger\right)\left(\omega_{TO,\perp}^2 - \omega_q^2\right)\left(\omega_{TO,\parallel}^2 - \omega_q^2\right)}$$

$$\text{x}\{[\epsilon(0)_\perp - \epsilon(\infty)_\perp]\omega_{TO,\perp}^2(\omega_{TO,\parallel}^2 - \omega_q^2)^2 sin^2\theta$$

$$+[\epsilon(0)_\parallel - \epsilon(\infty)_\parallel]\omega_{TO,\perp}^2\left(\omega_{TO,\perp}^2 - \omega_q^2\right)^2 cos^2\theta\}^{-\frac{1}{2}} \tag{63}$$

$$H = \sum_q(-e)\phi(q)e^{iqr}\left(a_q + a_{-q}^\dagger\right) \tag{64}$$

$$= i\sum_q\left\{\frac{4\pi e^2\hbar V^{-1}}{\left(\frac{\partial}{\partial w}\right)[\epsilon(\omega)_\perp sin^2\theta + \epsilon(\omega)_\parallel cos^2\theta}\right\}^{\frac{1}{2}}\frac{1}{q}e^{iqr}\left(a_q + a_{-q}^\dagger\right) \tag{65}$$

$$H_{Fr} = -i\sqrt{\frac{2\pi e^2\hbar\omega_{LO}}{V}\left[\frac{1}{\epsilon(\infty)} - \frac{1}{\epsilon(0)}\right]}\sum_q \frac{1}{q}(a_q e^{iq.r} - a_q^{\dagger} e^{-iq.r}) \quad (66)$$

2.2.3 Elastic Continuum Model

The elastic continuum models of phonons are used to well describe the acoustic phonons. It models the acoustic phonons of confined nanostructures of two atomic monolayers. From Hooke's law " T=Ye where Y is the proportionality constant also known as youngs modulus". Consider an element dx between x and x+dx along a structure. U(x,t) is the elastic displacement along the x axis of a 1-D structure. Strain is given as e=du/dx. The force is given by Newton's second law:

$$\rho(x)Adx\frac{\partial^2 u(x,t)}{\partial t^2} = [T(x+dx) - T(x)]A \quad (67)$$

$$T(x+dx) - T(x) = \left(\frac{\partial T}{\partial x}\right)dx = \left(\frac{Y\partial e}{\partial x}\right)dx = \left(Y\frac{\partial^2 u}{\partial x^2}\right)dx \quad (68)$$

the S_j are given by

$$S_1 = S_{xx} = \frac{\partial u}{\partial x},\ S_2 = S_{yy} = \frac{\partial v}{\partial y}, \qquad S_3 = S_{zz} = \frac{\partial w}{\partial z} \quad (69)$$

$$S_4 = S_{yz} = S_{zy} = \frac{1}{2}\left(\frac{\partial w}{\partial y} + \frac{\partial v}{\partial z}\right) \quad (70)$$

$$S_5 = S_{xz} = S_{zx} = \frac{1}{2}\left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x}\right) \quad (71)$$

$$S_6 = S_{xy} = S_{yx} = \frac{1}{2}\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right) \quad (72)$$

and T_i are of

$$T_1 = T_{xx};\ T_2 = T_{yy};\quad T_3 = T_{zz};$$

$$T_4 = T_{yz} = T_{zy};\qquad T_5 = T_{xz} = T_{zx};\quad T_6 = T_{xy} = T_{yx};$$

for $c_{ij}=c_{ji,}$ therefore instead of 36, only 21 unique elements are necessary to define the 6 x 6 matrix of c_{ij}. For example in cubic crystal

$$\begin{pmatrix} c_{11} & c_{12} & c_{12} & 0 & 0 & 0 \\ c_{12} & c_{11} & c_{12} & 0 & 0 & 0 \\ c_{12} & c_{12} & c_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{44} \end{pmatrix}$$

in wurzite crystal

$$\begin{pmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\ c_{12} & c_{11} & c_{13} & 0 & 0 & 0 \\ c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & (c_{11-}c_{12})/2 \end{pmatrix}$$

However, for zincblende crystal, only 3 distinct elements are needed c_{11}. c_{22} and $c_{44.}$ For isotropic cubic medium, the c_{ij} can be represented using two constants lambda and mu which are known as Lame's constant

$$\lambda = c_{12} = c_{13} = c_{21} = c_{23} = c_{31} = c_{32} \tag{73}$$

$$\mu = c_{44} = c_{55} = c_{66} = \frac{1}{2}(c_{11} - c_{12}) \tag{74}$$

$$\lambda + 2\mu = c_{11} = c_{22} = c_{33} \tag{75}$$

it follows that for an isotropic case we have

$$T_{xx} = \lambda\left(S_{xx} + S_{yy} + S_{zz}\right) + 2\mu S_{xx} = \lambda\nabla + 2\mu S_{xx},$$

$$T_{yy} = \lambda\left(S_{xx} + S_{yy} + S_{zz}\right) + 2\mu S_{yy} = \lambda\nabla + 2\mu S_{yy},$$

$$T_{zz} = \lambda\left(S_{xx} + S_{yy} + S_{zz}\right) + 2\mu S_{zz} = \lambda\nabla + 2\mu S_{zz},$$

$$T_{yz} = \mu S_{yz}, \quad T_{zx} = \mu S_{zx}\,, \quad T_{xy} = \mu S_{xy} \tag{76}$$

three dimensional generalizations are given by

$$\rho\frac{\partial^2 u}{\partial t^2} = \frac{\partial T_{xx}}{\partial x} + \frac{\partial T_{yx}}{\partial y} + \frac{\partial T_{zx}}{\partial z} = (\lambda + \mu)\frac{\partial \Delta}{\partial x} + \mu\nabla^2 u \tag{77}$$

$$\rho\frac{\partial^2 v}{\partial t^2} = \frac{\partial T_{xy}}{\partial x} + \frac{\partial T_{yy}}{\partial y} + \frac{\partial T_{zy}}{\partial z} = (\lambda + \mu)\frac{\partial \Delta}{\partial y} + \mu\nabla^2 v \tag{78}$$

$$\rho\frac{\partial^2 w}{\partial t^2} = \frac{\partial T_{xz}}{\partial x} + \frac{\partial T_{yz}}{\partial y} + \frac{\partial T_{zz}}{\partial z} = (\lambda + \mu)\frac{\partial \Delta}{\partial z} + \mu\nabla^2 w \tag{79}$$

The three force equation is also given as

$$\rho\frac{\partial^2 u_\propto}{\partial t^2} = \frac{\partial T_{\alpha\beta}}{\partial r_\beta} \tag{80}$$

where,

$$T_{\alpha\beta} = \lambda S_{\alpha\alpha}\delta_{\alpha\beta} + 2\mu S_{\alpha\beta} \tag{81}$$

The solutions for the displacement field of acoustics are described in terms of potential function, through

$$u = \frac{\partial \phi}{\partial x} + \frac{\partial \Psi_x}{\partial x} - \frac{\partial \Psi_y}{\partial z} \tag{82}$$

$$v = \frac{\partial \phi}{\partial y} + \frac{\partial \Psi_x}{\partial z} - \frac{\partial \Psi_y}{\partial x} \tag{83}$$

$$w = \frac{\partial \phi}{\partial z} + \frac{\partial \Psi_y}{\partial x} - \frac{\partial \Psi_x}{\partial y} \tag{84}$$

where

$$\nabla^2 \phi = \frac{1}{c_l^2} \frac{\partial^2 \phi}{\partial t^2} \tag{85}$$

$$\nabla^2 \Psi_i = \frac{1}{c_t^2} \frac{\partial^2 \Psi_i}{\partial t^2}; \;\; i = x, y, z \tag{86}$$

$$c_l^2 = (\lambda + 2\mu)/\rho \tag{87}$$

$$c_t^2 = \lambda/\rho \tag{88}$$

The non-rotational solution is referred to as longitudinal acoustic modes and rotational is referred to as transverse mode

CHAPTER 3 ANHARMONIC DECAY OF PHONONS IN BULK CRYSTALS

3.1 Anharmonic Decay

The phonon vibration in crystal is assumed to be that of a harmonic oscillator, however there are higher order terms that represent anharmonic interactions which are important to describe the process of phonon decay. The crystal potential is given by Taylor expansion series with quadratic terms and higher order terms. The quadratic term represents the two phonon process, which are harmonic. The higher order term for example the cubic term represents the three phonon process as shown in figure [3]. Considering the the three phonon process in which an optical phonon decays into two acoustical phonons. The cubic term can be written as

$$H'_{q,j;q\prime,j\prime;q\prime\prime,j\prime\prime} = \frac{1}{\sqrt{N}} P(q,j;q',j';q'',j'') u_{q,j} u_{q\prime,j\prime} u_{q\prime\prime,j\prime\prime} \tag{89}$$

Where $u_q$represents the displacement optical phonon which was annihilated and $u'_q \; and \; u''_q$ are the displacements of two acoustical phonons created.

3.2 Klemens Channel

The anharmonic decay of the zone center LO phonons have been well studied theoretically and experimentally [1],[10] and [20]. The longitudinal optical phonons have the highest energy among all phonon types, so the decay process of this longitudinal optical phonon mode could be

into two low energies acoustical phonon or a TO and LA. Klemens (1966) [1] predicts that the zone center longitudinal optical (LO) phonons can decay into two transverse acoustical(TA) or longitudinal acoustical (LA) phonons like LO=LA+LA or LO= TA+TA, which is termed Klemens Channel, as shown in Figure [4] and [5]

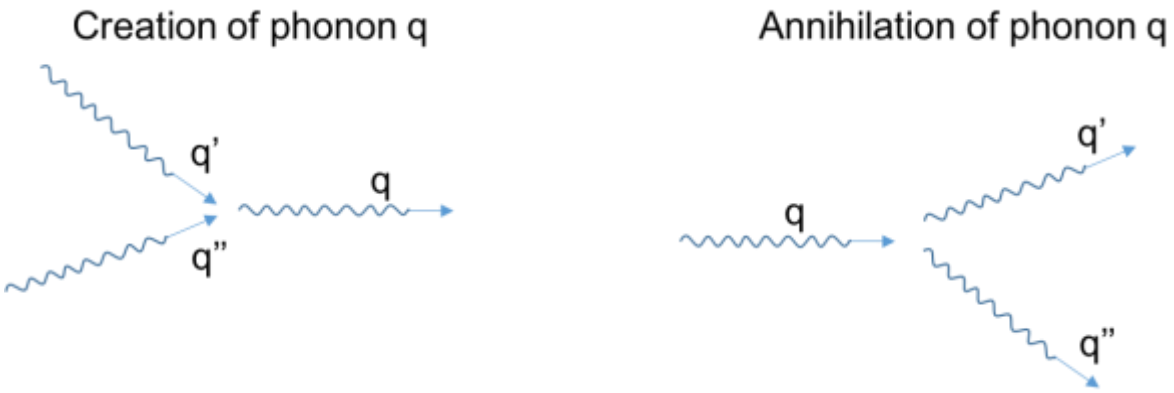

Figure 3:The three-phonon process of phonons

$$K_{LO} = K_{LA1} + K_{LA2} \tag{90}$$

$$H'_{q,j;q',j';q'',j''} = \frac{1}{\sqrt{N}}{}^{3}\sqrt{\frac{\hbar}{2m}}\left(\frac{1}{\omega_q \omega_{q'} \omega_{q''}}\right)^{\frac{1}{2}} P(q,q',q'') a_q a^{\dagger}_{q'} a^{\dagger}_{q''} e^{i(q-q'-q'')} \tag{91}$$

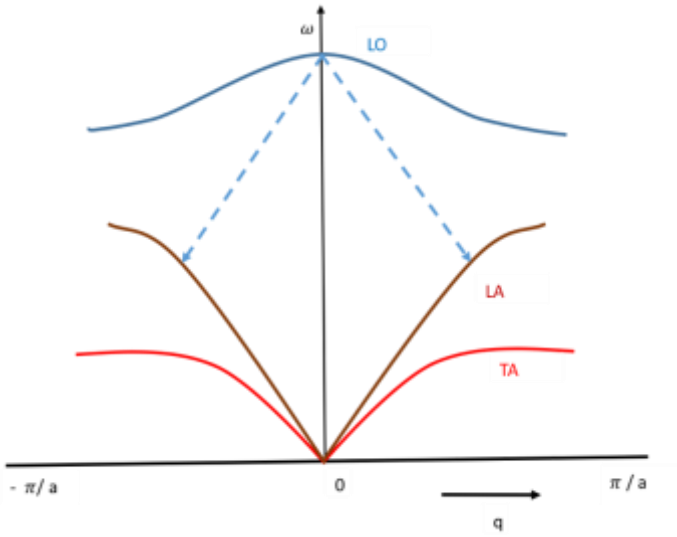

Figure 4: LO phonon decay into two LA phonons

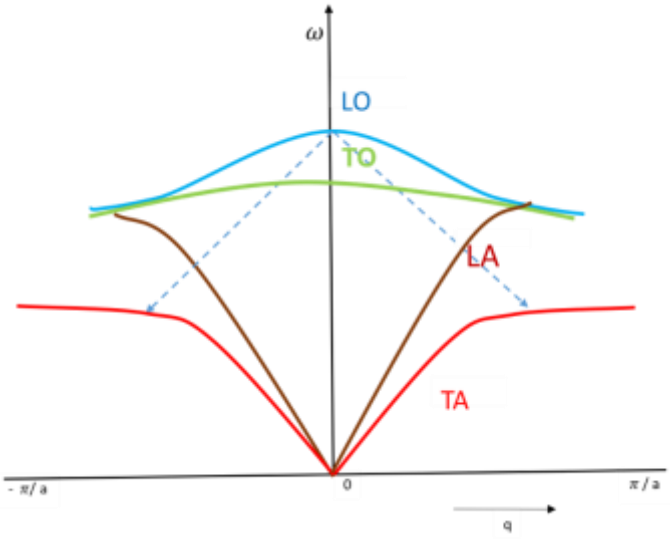

Figure 5: LO phonon decay into two TA phonons

3.3 Ridley Channel

In 1996, Ridley discussed the same scenario in GaN. The LO phonons of GaN is greater than twice the LA phonon energy therefore the LO=LA+LA is not feasible. Therefore, the decay process is give by LO-> TO+LA/TA. This process is called Ridley channel.

TO phonons has also been studied and the decay is only through two acoustic phonons in case of Ridley decay channel. [11]

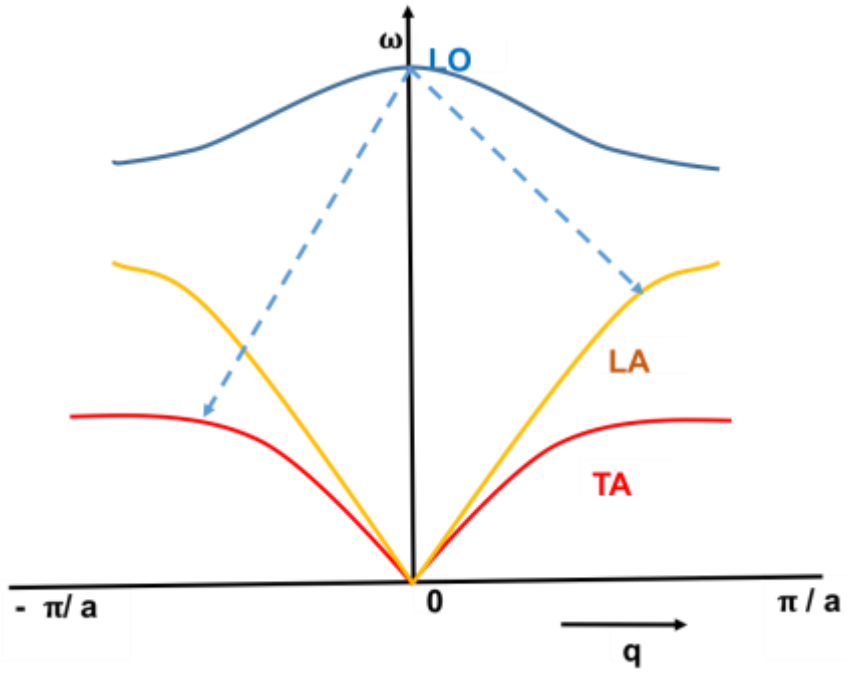

Figure 6: Ridley's channel, LO phonon decay into LA and TA phonons

3.4 Klemens Anharmonic decay and lifetime estimation

Klemens estimated the theoretical lifetime of anharmonic decay of optical phonon. In his work, he considered the optical phonon at q=0 of frequency ω_o which decays into two acoustical phonon by anharmonic process.

$$\omega_o = \omega' + \omega'' \tag{92}$$

and momentum,

$$q = q' + q'' = 0 \tag{93}$$

$$H' = \sum_{q,q',q''} \frac{1}{G} e^{i(q-q'-q'').x_c(q,q',q'')} \times a(q)a^*(q')a^*(q'') \tag{94}$$

from standard perturbation theory,

$$t\frac{dN}{dt} = 2\sum_{j',j'',q'} \frac{c^2\hbar^3}{M^3\omega\omega'\omega''} \frac{1-cos\Delta\omega t}{\Delta\omega^2} \tag{95}$$

$$\times [(N+1)N'N'' - N(N'+1)(N''+1)]$$

$$\frac{1}{\tau} = -\frac{1}{n}\frac{dN}{dt} \tag{96}$$

$$\frac{1}{\tau} = \omega_0 \frac{J}{24\pi}\gamma^2 \frac{\hbar\omega_0}{Mv^2}\frac{a^3\omega_0^3}{v^3} \tag{97}$$

3.5 Lifetime of Optical phonon

Bhatt and Stroscio [12] studied the lifetime of longitudinal optical phonons(LO) in zinc blende semiconductors. Using the theory of elasticity, the crystal anharmonic potential is calculated based on this the lifetime of LO phonon which decays into two acoustical phonon is estimated as a function phonon wave vector and that of the lattice temperature.

The Hamiltonian of three phonon process is given by

$$H'_{q,j;q',j';q'',j''} = \frac{1}{\sqrt{N}} P(q,j;q',j;q'',j) u_{q,j} u_{q',j'} u_{q'',j''} \quad (98)$$

where $k, k'\ and\ k''$represent the phonon wave vector, P is the phonon coupling and N is the number of unit cells.

The displacement of the phonon is given by $u_{k,j}$

$$u_{q,j} = \left(\frac{\hbar}{2m\omega_{k,j}}\right)^{\frac{1}{2}} e'_{q,j}(a_{q,j} e^{iq.r} + a^{\dagger}_{q,j} e^{-iq.r}) \quad (99)$$

where $a_{k,j}\ and\ a^{\dagger}_{k,j}$ are the annihilation and creation operator respectively.

$e'_{k,j}$ is the polarization vector and m is the average mass of the lattice atoms

$$\frac{1}{m} = \frac{1}{M1} + \frac{1}{M2} \quad (100)$$

M1 and M2 mass of atom 1 and atom 2 in the crystal lattice.

The Hamiltonian for this process becomes

$$H'_{q,q',q''} = \frac{1}{\sqrt{N}} \left(\frac{\hbar}{2m}\right)^{3/2} \left(\frac{1}{\omega_q \omega_{q'} \omega_{q''}}\right)^{1/2} \times P(q,q',q'') a_q a^{\dagger}_{q'} a^{\dagger}_{q''} e^{i(q-q'-q'').r} \quad (101)$$

The matrix element was defined as

$$|M|^2 = \frac{\hbar^3 U_a^2}{8Nm^3} \left(\frac{1}{\omega_q \omega_{q'} \omega_{q''}}\right) n_q (n_{q'} + 1)(n_{q''} + 1) \delta_{q,q'+q''} \quad (102)$$

The transition rate is given by

$$\Gamma = \frac{2\pi}{\hbar}\sum_{q'q''}|M|^2\,\delta(\hbar\omega_q - \hbar\omega_{q'} - \hbar\omega_{q''}) \tag{103}$$

The lifetime of LO phonon was given by

$$\frac{1}{\tau_p} = \sum \frac{\pi\hbar^2 U_a^2}{4Nm^3}\left(\frac{1}{\omega_q\omega_{q'}\omega_{q''}}\right)(1 + n_{q'}+n_{q''})\delta_{q,q'+q''}\delta(\hbar\omega_q - \hbar\omega_{q'} - \hbar\omega_{q''}) \tag{104}$$

CHAPTER 4 LIFETIME OF CONFINED PHONONS IN GaAs

GaAs is a important semiconductor for technological improvements. They are of interest because they are used in the manufacturing of devices like IC's- high frequency IC's and various optimal diodes. In most these devices the decay rate of optical phonon play a major role, like the switching time of the laser depends on how rapidly the LO phonons decay into 100 times weaker acoustic phonons. Some properties of GaAs are superior to the properties of those of Si for example it has high saturated electron velocity and mobility, this aids in the functioning of transistors at slightly above 250 GHz frequencies. Because of these properties quantum devices are manufactured using GaAs therefore its of interest to study about the lifetime of phonons confined in these GaAs devices.

4.1 AlAs/GaAs/AlAs

The case of confined GaAs is considered to study the lifetime of confined phonons. To achieve the confinement, GaAs is sandwiched between the AlAs crystal. Therefore an ultrathin structure of GaAs(2D) is achieved, and phonons are confined in the confinement. This interface structure and the crystal structure has been explained in this section.

4.1.1 GaAs Crystal Structure

Gallium Arsenide is a polar semiconductor, which belongs to the elements gallium of group III and arsenic of group V making it III-V element with direct band gap semiconductor. The crystal structure of GaAs is zinc blende. It has ionic bonding which results in charge transfer from the Group V toms which have five electrons in the outer shell to the group III atoms which have three atoms in the outer shell. Therefore, gallium atoms receive net negative charge and the arsenic receives positive charge.

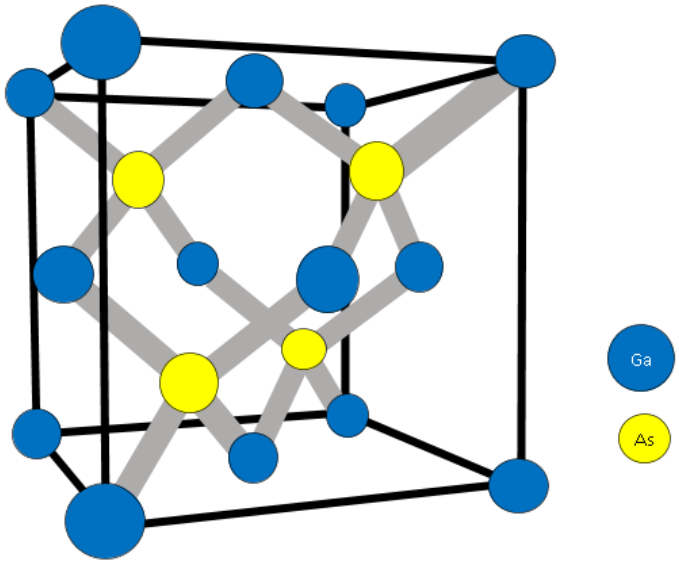

Figure 7: GaAs crystal structure.

4.1.2 Dispersion Relation of confined phonons in GaAs

A dispersion relation relates the wavelength of a wave with the frequency of the wave. For dispersion relation of bulk phonons has been explained in section [].

In dispersion relation of confined phonons, the curves are quantized with discrete points n=1,2,3… The dispersion relation of GaAs in brillouin zone is given by Bardeen and Shockley [9] as shown in figure.

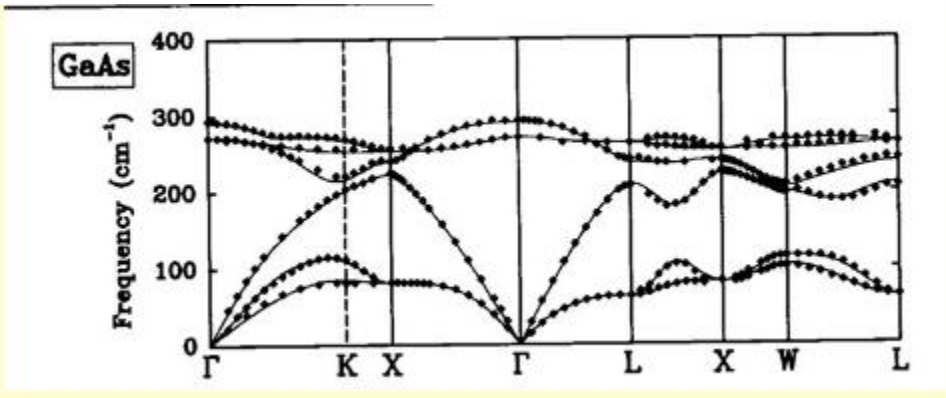

Figure 8: Dispersion curve of GaAs – Image from Bardeen and Shockley [9]

4.1.3 Double Heterointerface structures- AlAs/GaAs/AlAs

The interfaced that occurs between two layers of region of different crystal is called heterointerface. In AlAs/GaAs/AlAs, the GaAs is sandwiched between AlAs along the z direction as shown in figure [9] Thus the GaAs is confined in z direction however assumed to be infinite in the directions along x and y axis. Quantization of optical phonons affect the electrical, optical and thermal properties of ultra thin structures.

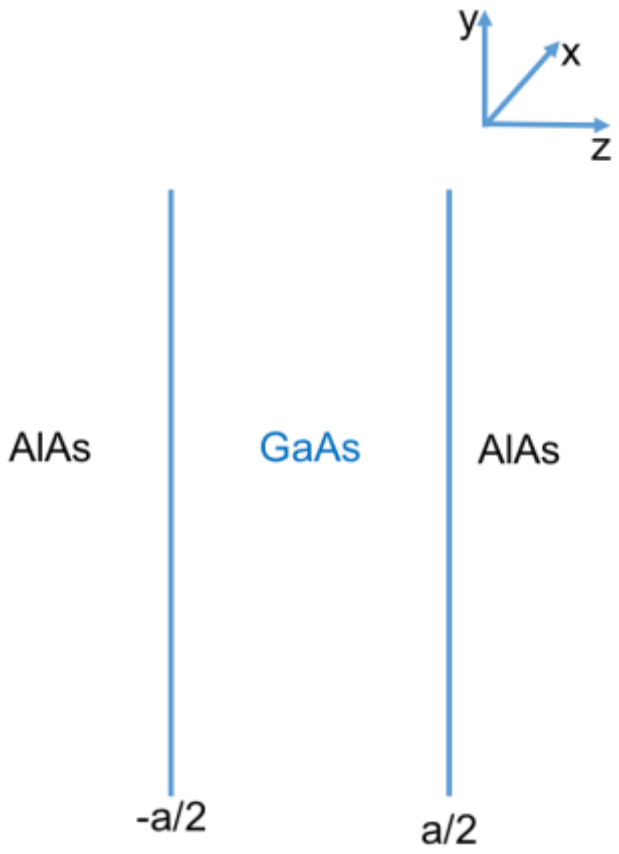

Figure 9: Double interface heterostructures

4.2 Anharmonic decay of optical phonons confined in GaAs

The optical phonons decays into two acoustical phonons in anharmonic decay as explained in sec[]. To study about the lifetime of optical phonon it is very important to consider is three phonon decay process.

4.2.1 Energy and momentum conservation

For the anharmonic decay process to occur in confined phonons, the energy and momentum should be conserved in this process. From the figure [8] and [10], we can see that the energy and momentum is conserved and is given by

$$\hbar\omega = \hbar\omega' + \hbar\omega'' \tag{105}$$

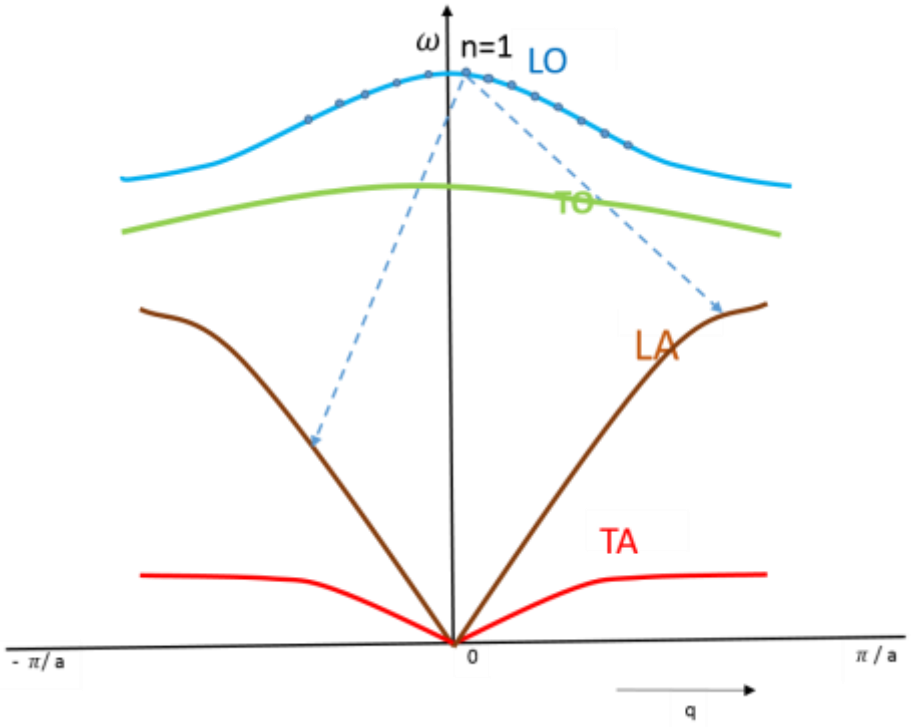

Figure 10: Decay of LO phonon in confined structure

4.3 Estimation of Lifetime of LO confined phonon

The interaction strength of this three-phonon process is given by Hamiltonian obtained from Taylor series expansion with quadratic, cubic and higher order terms. The quadratic term is generally considered for simplification however, the cubic or anharmonic term which represent

the three-phonon process is important for estimation of lifetime time of optical phonon. This is because most of the optical phonons decay into two acoustical phonons.

The Hamiltonian representing this process is given by

$$H'_{q,j;q',j';q'',j''} = \frac{1}{\sqrt{N}} P(q,j;q',j;q'',j) u_{q,j} u_{q',j'} u_{q'',j''} \tag{106}$$

where $P(q,j;q',j;q'',j)$ represents the anharmonic coupling coefficient, $u_{q,j}, u_{q',j'}, u_{q'',j''}$ are the displacement of the optical phonon and two acoustic phonons involved in the anharmonic decay process respectively.

The interface mode's optical phonon displacement in the AlAs/GaAs/AlAs structure is given by the transfer matrix model of multi interface hetero structure [14]. The displacement is related to the electric polarization which is given by

$$u_i(q,z) = \frac{P_i(q,z)}{n_i e_i^* [1+\alpha_i \mu_i e_i^{*-2} (\omega_{0i}^2 - \omega^2)]} \tag{107}$$

where $P_i(q,z)$ is the electric polarization, it follows

$$P_i(q,z) = -\chi_i(\omega)[iq\Phi_i(q,z)\hat{q} + \frac{\partial \Phi_i(q,z)}{\partial z}\hat{z}] \tag{108}$$

it follows that

$$u_i(q,z) = \frac{-\chi_i(\omega)[iq\Phi_i(q,z)\hat{q} + \frac{\partial \Phi_i(q,z)}{\partial z}\hat{z}]}{n_i e_i^* [1+\alpha_i \mu_i e_i^{*-2} (\omega_{0i}^2 - \omega^2)]} \tag{109}$$

$\Phi_i(q,z)$ is the carrier-optical phonons interaction's electrostatic potential which is given as

$$\Phi_i(q,z) = A(c_{i-} e^{-qz} + c_{i+} e^{+qz}) = A\varphi_i(q,z) \tag{110}$$

where A is the normalization constant given by

$$A = \left(\frac{\hbar}{2\omega L^2}\right)^{1/2} \left(\sum_i \frac{1}{4\pi}\frac{1}{2\omega}\frac{\partial \epsilon_i(\omega)}{\partial \omega} \times \int dz \left\{q^2|\varphi_i(q,z)|^2 + \left|\frac{\partial \varphi_i(q,z)}{\partial z}\right|^2\right\}\right)^{-1/2} \quad (111)$$

In the case of AlAs/GaAs/AlAs of thickness a (z=-a/2 to +a/2), the phonon potential decreases exponentially for z tending to infinity and the phonon potential in the quantum well is a combination of increasing and decreasing exponentials. Considering even potential, the dielectric constant in the quantum well is $\epsilon_1(\omega)$ and the AlAS as $\epsilon_2(\omega)$.

Then,

$$\Psi_0(q,z) = e^{+q\left(z+\frac{a}{2}\right)} \; for \; z \leq -\frac{a}{2} \quad (112)$$

$$\Psi_1(q,z) = \frac{2coshqz}{coshqa} \; for \; |z| < \frac{a}{2} \quad (113)$$

$$\Psi_2(q,z) = e^{+q\left(z+\frac{a}{2}\right)} \; for \; z \geq \frac{a}{2} \quad (114)$$

represents the envelope for the phonon potential.

It follows that,

$$\int_{R0} dz \left(q^2|\Psi_0(q,z)|^2 + \left|\frac{\partial \Psi_0(q,z)}{\partial z}\right|^2\right) = q \quad (115)$$

$$\int_{R1} dz \left(q^2|\Psi_1(q,z)|^2 + \left|\frac{\partial \Psi_1(q,z)}{\partial z}\right|^2\right) = 2q \; tanhqd/2 \quad (116)$$

$$\int_{R2} dz \left(q^2 |\Psi_2(q,z)|^2 + \left| \frac{\partial \Psi_2(q,z)}{\partial z} \right|^2 \right) = q \tag{117}$$

substituting the above equation in A we get

$$A = \left(\frac{\hbar}{2\omega L^2} \right)^{1/2} \left[\frac{1}{2\omega} \frac{\partial \epsilon_0(\omega)}{\partial \omega} 2q + \frac{1}{2\omega} \frac{\partial \epsilon_1(\omega)}{\partial \omega} 2qtanh \frac{qd}{2} \right]^{-1/2} \tag{118}$$

The acoustic phonons in double interface heterostructures

is given by Wendler and Grigoryan (1988) [13]. They classified the acoustic modes as symmetric shear horizontal waves and antisymmetric shear horizontal waves.

$$u(x,y,z) = u(z).\exp[i(q_{\parallel}x - \omega t)] \tag{119}$$

the shear vertical (SV) modes with two non-zero component is given as

$$u(z) = (u_1(z), 0, u_3(z)) \tag{120}$$

and shear horizontal (SH) modes with one non-zero component

$$u(z) = (0, u_2(z), 0) \tag{121}$$

For symmetric modes

$$u_i(z) = u_i(-z) \tag{122}$$

For antisymmetric modes

$$u_i(z) = -u_i(-z) \tag{123}$$

the displacement of Symmetrical shear waves(SSV) is given by

$$u_1^s(z) = \begin{cases} A_2^s \exp(-\eta_{l2} z) + B_2^s \exp(-\eta_{t2} z) & z > a/2 \\ A_1^s \cosh\eta_{l1} z + B_1^s \cosh\eta_{t1} z & \frac{a}{2} > z > -\frac{a}{2} \\ A_2^s \exp(\eta_{l2} z) + B_2^s \exp(\eta_{t2} z) & z < -a/2 \end{cases} \tag{124}$$

$$u_3^s(z) = \begin{cases} i\left[\frac{\eta_{l2}}{q_\parallel} A_2^s \exp(-\eta_{l2} z) + \frac{q_\parallel}{\eta_{t2}} B_2^s \exp(-\eta_{t2} z\right] & z > \frac{a}{2} \\ i\left[\frac{\eta_{l1}}{q_\parallel} A_1^s \sinh\eta_{l1} z - \frac{q_\parallel}{\eta_{t1}} B_1^s \sinh\eta_{t1} z\right] & \frac{a}{2} > z > -\frac{a}{2} \\ i\left[\frac{\eta_{l2}}{q_\parallel} A_2^s \exp(\eta_{l2} z) - \frac{q_\parallel}{\eta_{t2}} B_2^s \exp(\eta_{t2} z)\right] & z < -\frac{a}{2} \end{cases} \quad (125)$$

The displacement of Antisymmetric shear vertical modes is given by

$$u_1^A(z) = \begin{cases} A_2^A \exp(-\eta_{l2} z) + B_2^A \exp(-\eta_{t2} z) & z > a/2 \\ A_1^A \sinh\eta_{l1} z + B_1^s \sinh\eta_{t1} z & \frac{a}{2} > z > -\frac{a}{2} \\ A_2^A \exp(\eta_{l2} z) + B_2^A \exp(\eta_{t2} z) & z < -a/2 \end{cases} \quad (126)$$

$$u_3^A(z) = \begin{cases} i\left[\frac{\eta_{l2}}{q_\parallel} A_2^A \exp(-\eta_{l2} z) + \frac{q_\parallel}{\eta_{t2}} B_2^A \exp(-\eta_{t2} z)\right] & z > \frac{a}{2} \\ i\left[-\frac{\eta_{l1}}{q_\parallel} A_1^A \cosh\eta_{l1} z - \frac{q_\parallel}{\eta_{t1}} B_1^A \cosh\eta_{t1} z\right] & \frac{a}{2} > z > -\frac{a}{2} \\ i\left[\frac{\eta_{l2}}{q_\parallel} A_2^A \exp(\eta_{l2} z) - \frac{q_\parallel}{\eta_{t2}} B_2^A \exp(\eta_{t2} z)\right] & z < -\frac{a}{2} \end{cases} \quad (127)$$

Where

$\eta_{li} = ({q_\parallel}^2 - \frac{\omega^2}{c_{li}^2})^{1/2}$ and $\eta_{ti} = ({q_\parallel}^2 - \frac{\omega^2}{c_{ti}^2})^{1/2}$

The shear horizontal modes are given as

SSH modes:

$$u_2^S(z) = \begin{cases} D_2^S \exp(-\eta_{t2} z) & z > a/2 \\ D_1^S \cos\theta_{t1}\, z) & \frac{a}{2} > z > -\frac{a}{2} \\ D_2^S \exp(-\eta_{t2} z) & z < -a/2 \end{cases} \quad (129)$$

and ASH modes,

$$u_2^A(z) = \begin{cases} D_2^A \exp(-\eta_{t2} z) & z > a/2 \\ D_1^A \sin\theta_{t1}\, z) & \frac{a}{2} > z > -\frac{a}{2} \\ -D_2^A \exp(-\eta_{t2} z) & z < -a/2 \end{cases} \quad (130)$$

where,

$$\theta_{t1} = i\eta_{t1}$$

from the Fermi golden rule, we have, the transition probability also known as decay probability which is related to the inverse of the mean lifetime [15].

In general,

$$\Gamma = \frac{2\pi}{\hbar} |\langle f|H'|i\rangle|^2 \rho \quad (131)$$

Where, $\langle f|H'|i\rangle$ is the matrix element

For a phonon process

$$\frac{1}{\mathrm{T}} = \frac{2\pi}{\hbar} \left|\left\langle n_{phonon} \pm 1 \middle| H' \middle| n_{phonon} \pm 1 \right\rangle\right|^2 \rho \quad (132)$$

Where $\langle n|a^+|n\rangle = \sqrt{n+1}\sqrt{\frac{\hbar}{2m\omega}}$

the matrix element of a three phonon process is given by,

$$M = \langle n_q^f, n_{q'}^f, n_{q''}^f | H' | n_q^i, n_{q'}^i, n_{q''}^i \rangle \quad (133)$$

Considering the entire phonon decay process in a crystal, Matrix element average with boundary condition $q_y = \pm \frac{m\pi}{L_y} and\ q_z = \pm \frac{n\pi}{L_z}$

$$M_{avg}^2 = \frac{1}{a} \int_{-\frac{a}{2}}^{\frac{a}{2}} cos^2(q_z z) dz \quad (134)$$

$$M_{avg}^2 = 1/2 \quad (135)$$

therefore, the decay rate of optical phonon confined in the quantum well is half of the mean decay rate of the unconstrained phonon.

CHAPTER 5 CONCLUSION

5.1 Comparison with bulk phonon

From the above equation, we can conclude that the lifetime of confined phonon is twice the lifetime of phonon in bulk crystals.

5.2 Conclusion

The lifetime of optical phonon is doubled by the confinement; this makes the confinement better in the manufacturing of semiconductor device. Since the decay rate of phonons is reduced, the lifetime of optical phonon is more. Thus the optical phonon decay slower into acoustical phonons which are much weaker than optical phonon.

CHAPTER 6 INDUSTRY LEARNINGS ON THE IMPORTANCE OF PHONONS IN CONFINED STRUCTURES

6.1 Industry exposure

One of the vast field that as moved to the nanoscale is VLSI. For further reduction by few nanometer, there are property changes or limitation of nanoscience. At Intel, I worked as Physical Design engineer to understand the various problems faced while designing the chip and during fabrication. In this role, I worked from RTL to GDS of the ASIC design. The Physical design flow is as follows - Synthesis, Placement, routing, Clock tree synthesis, Timing, DRC, LVS, RC extraction, GDS and tape out. I also got the chance to work on the analysis of the chip like IR drop, Signal EM and Power EM.

Synthesis is where the RTL netlist is obtained from the designers and then with the help of tools the netlist is synthesized to gate level netlist which is then placed on the chip and routing is done. After which the clock tree is built and accurate timing is calculated. The timing check includes the setup time and hold time analysis. Then the DRC check and the LVS check is performed on the design. The design is then validated in Redhawk for hotspots, IR Drop and EM checks.

6.2 Issues faced in VLSI

On working at Intel, I got an insight of the major problems in very large scale integrations. The current technology used in the industries are between 10nm and 28nm. The technology defines

the channel width or the smallest feature of the design on the chip. The Moore' s law states that the number of transistors doubles every year.

As the transistor density of the chip keeps increasing we hit certain limitations due to the following issues. The power required for the chip in a small area increases, leading to failure of the IR drop. <need to add more on hotspot> However, the most important checks for a chip to tape-out is the DRC check and Timing requirements to be met which becomes more and more difficult as we scale down a few nanometers. Also, there are fabrication issues due to scaling which leads to increased design rule checks.

6.3 How phonons play a role

As we have discussed earlier, the phonons play a major role on the operating speed of the device as the carrier mobility of electrons depends on phonons. The design constraints of the chip is used determine the timing requirements. In turn the design constraints are dependent on the frequency the chip is going to be operated on. Each cells in the design contribute to a delay due to its switching speed. Phonons determine the carrier mobility or the switching speed of the device. A small improvement on the switching speed of the device would cause huge impact in the industry as timing is one of the most essential check for tape out.

Also, the acoustic phonons determine the heat transport in the material. Another major issue is the hotspots in the design.

Thus, this study about lifetime of phonons in confined structures is very important to overcome the obstacle of scaling down the chip as described in the Moore's law.

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APPENDIX

Fermi-golden rule

Fermi's Golden rule is an equation to estimate the probability of transition per unit time or constant transition rate from initial state to final state of a quantum system. It provides a perturbative result to estimate phonon-phonon interaction rate or carrier-phonon interaction rate.

Consider an unpertubated system with Hamiltonian H and in eigenstate, $|i\rangle$ and the effect of a pertubated Hamiltonian H'. There are two cases for H', which is time-independent and time-dependent. In the case of time independent H', the system goes only to continuum states that have energy equal to the initial state. In cases where H' is time dependent with angular frequency ω, the system goes to states with energies that changes by $\hbar\omega$ from the initial state.

However, the transition probability from initial state $|i\rangle$ to final states $|f\rangle$ per unit of time is a constant. It is given by the first order of perturbation as follows

$$\Gamma_{i\to f} = \frac{2\pi}{\hbar}|\langle f|H'|i\rangle|^2\rho$$

Where, ρ is the density of final state

$|\langle f|H'|i\rangle|^2$ is the square of the matrix element or $|M|^2$

APPENDIX (Continued)

Since in transition the phonon decays the transition probability is also know as the decay probability, inverse of which is the mean lifetime.

Derivation for computing the lifetime of phonons

For a phonon process

$$\frac{1}{\mathrm{T}} = \frac{2\pi}{\hbar}\left|\left\langle n_{phonon} \pm 1\middle|H'\middle|n_{phonon} \pm 1\right\rangle\right|^2 \tag{132}$$

Where $\langle n|a^+|n\rangle = \sqrt{n+1}\sqrt{\frac{\hbar}{2m\omega}}$

the matrix element of a three phonon process is given by,

$$M = \left\langle n_q^f, n_{q'}^f, n_{q''}^f\middle|H'\middle|n_q^i, n_{q'}^i, n_{q''}^i\right\rangle \tag{133}$$

Considering the entire phonon decay process in a crystal, Matrix element average with boundary condition $q_y = \pm\frac{m\pi}{L_z} and\ q_z = \pm\frac{n\pi}{L_z}$

$$M_{avg}^2 = \frac{1}{a}\int_{-\frac{a}{2}}^{\frac{a}{2}} cos^2(q_z z)dz \tag{134}$$

$$= \frac{1}{a}\int_{-\frac{a}{2}}^{\frac{a}{2}} cos^2(q_z z)dz$$

$$= \frac{1}{a}\int_{-\frac{a}{2}}^{\frac{a}{2}} \frac{1+cos2q_z z}{2}dz$$

APPENDIX (Continued)

$$= \frac{1}{2a}\int_{-\frac{a}{2}}^{\frac{a}{2}} 1 + cos2q_z z dz$$

$$= \frac{1}{2a}\left[z + \frac{\sin 2q_z z}{2q_z}\right]_{-\frac{a}{2}}^{\frac{a}{2}}$$

$$= \frac{1}{2a}\left[\frac{a}{2} + \frac{a}{2}\right]$$

$$= \frac{1}{2a}[a]$$

$$M_{avg}^2 = 1/2 \quad (135)$$

therefore, the lifetime of optical phonon confined in the quantum well is half of the mean lifetime of the unconstrained phonon.

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