

Electron – Phonon Interaction in Emerging Semiconductors

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THESIS

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SUMMARY

This thesis is an investigation of the quantized normal mode of vibrations of the constituent atoms of semiconductors, referred to as phonons, and its effect on carrier transport and thermal conductivity of emerging semiconductors. Interaction of charge carriers with phonons is the dominant mechanism through which charge carriers exchange energy with the crystal lattice, hence their proper understanding becomes of prime importance while modelling carrier transport in a semiconductor. The phonon modes undergo significant modification as a result of dimensional confinement or presence of interfaces in semiconductors which must be taken into account while modelling their interaction with charge carriers. The carrier phonon interaction and phonon decay mechanisms are the main topic of study in this thesis applied to the case of emerging semiconductors which are wide band gap and in which electrons couple very strongly to the optical phonons. These emerging semiconductors are finding wide application in high power and high frequency applications. The main findings of this study are:

- (1) Surface acoustic phonon modelling by quantization of Rayleigh waves on the diamond surface has been done and its interaction with holes present in two dimensional hole gas on the surface has been performed.
- (2) A novel heterostructure consisting of cubic Boron Nitride and Diamond has been investigated to be used as a High Electron Mobility Transistor. Conditions of production of two dimensional electron gas and its interaction with surface acoustic phonons and remote polar phonon has been studied.

SUMMARY (Continued)

- (3) Modelling of acoustic phonon decay through three phonon process has been done for wurtzite crystals duly accounting for its anisotropy. Such study is fundamental for evaluation of thermal conductivity of the crystals.
- (4) Electric field velocity relations and other transport parameters have been evaluated for technologically important wurtzite and emerging cubic crystals under the purview of path integral mechanism (Thornber – Feynman polaron theory). The traditional relaxation time approach based on perturbative techniques breaks down in these materials which warrants use of non-perturbative path integral techniques. Correction factors have been obtained for Fermi's golden rule to properly account for mobility of charge carriers.
- (5) Thornber – Feynman's polaron theory has been extended to emerging two dimensional Transition Metal Di-Chalcogenides. It is demonstrated that Fermi's golden rule breaks down in these strongly coupled materials. Electric field – velocity relations have been worked out along with carrier mobility.
- (6) Role of confined optical phonons is investigated in exciton generation for a quantum dot interacting with laser modelled as a classical light. This study forms a basis for qubit state preparation in quantum computing applications.

Chapter 1

Introduction

1.1 Background

The constituent atoms in any semiconductor solid don't have static physical location, rather they exhibit periodic motion about their equilibrium position. Since, the atomic cores are much heavier relative to the electrons, therefore the Adiabatic approximation enables us to treat the motion of atomic cores independently of the electrons. The crystal potential energy attributed to the interatomic pair potential can be expanded in a Taylor series as shown below:

$$U(x) = U(a_0) + \left(\frac{\partial U}{\partial a}\right)_{a=a_0} x + \frac{1}{2} \left(\frac{\partial^2 U}{\partial a^2}\right)_{a=a_0} x^2 + \dots \quad (1.1)$$

where, a and a_0 represents the instantaneous interatomic separation, a_0 is the equilibrium position and $x = a - a_0$. Since, $\left(\frac{\partial U}{\partial a}\right)_{a=a_0} = 0$ so we can approximate the crystal potential energy according to harmonic approximation, such that $\left(\frac{\partial^2 U}{\partial a^2}\right)_{a=a_0}$ is referred to as interatomic force constant. This enables us to model the ion core motion by a linear chain model (which can be generalized to a 3-dimensional picture), as shown below:

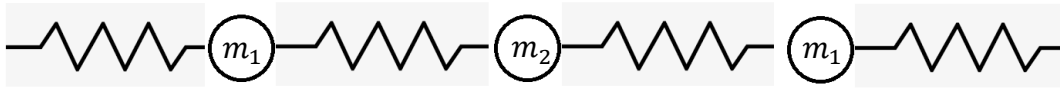


Fig. 1.1 1d linear chain model

The normal modes of vibration representing the atomic displacements (longitudinal displacements along the chain) of mass m_1 and m_2 in Fig.1 can be written as:

$$u_{2r} = A_1 \exp i(2rqa - \omega t) \quad (1.2)$$

and,

$$u_{2r+1} = A_2 \exp i((2r + 1)qa - \omega t) \quad (1.3)$$

where, q is the wave vector and $A_{1,2}$ represents the amplitude of mass $m_{1,2}$. Let κ be the inter atomic force constant. The restoring force on each mass can be represented by Hooke's law: $F_{res} = -\kappa x$. Using Eq. (2) and (3), we apply newton's second law of motion on each mass and further eliminate A_1 and A_2 from the resulting equations, the final expression expressing relation between the wave vector q and the frequency ω can be written as [1]:

$$\omega^2 = \kappa \left(\frac{1}{m_1} + \frac{1}{m_2} \right) \pm \kappa \left[\left(\frac{1}{m_1} + \frac{1}{m_2} \right)^2 - \frac{4 \sin^2 qa}{m_1 m_2} \right]^{1/2} \quad (1.4)$$

The high frequency solution of Eq. (4) is referred to as longitudinally optical (LO) mode, (as for many semiconductors its value lies in terahertz region which corresponds to the infra red portion of the electromagnetic spectrum) whereas the low frequency solution is called as longitudinally acoustic (LA) mode. The energies of such normal modes of vibration are quantized which is given as:

$$E_n = \left(N_q + \frac{1}{2} \right) \hbar \omega_q \quad (1.5)$$

where, N_q is the Bose – Einstein phonon occupation number, given as below:

$$N_q = \frac{1}{\exp \left(\frac{\hbar \omega_q}{k_{BT}} \right) - 1} \quad (1.6)$$

N_q determines the number of phonon modes of frequency ω_q with a wave vector $\mathbf{q}$. Such vibrational normal modes having quantized energy are referred to as *phonons*. These phonons carry a momentum $\hbar \mathbf{q}$.

1.2 Phonons in polar semiconductors

The atoms of semiconductors are bonded covalently with the neighbouring atoms, however for compound semiconductors in which the constituent atoms belong to different group in the periodic table the nature of bond has more ionic character as the atoms are further separated in periodic table [2], for example, II-VI semiconductor CdSe has more ionic bond as compared to III-V semiconductor GaAs. The discussion in the following paragraph motivates the production of polarization $\mathbf{P}$ due to phonon modes in a compound semiconductor which forms a basis for modelling electron – phonon interaction mechanism to be explained in later sections.

Let e^* and $-e^*$ be the charge on mass m_1 and m_2 in the diatomic linear chain model in the previous section. The force equations on both the masses can be written as [1]:

$$\begin{aligned} m_1 \frac{d^2 u_{2r}}{dt^2} &= -m_1 \omega^2 u_{2r} = \kappa(u_{2r+1} + u_{2r-1} - 2u_{2r}) + e^* E \\ &= \kappa(e^{i2qa} + 1)u_{2r+1} - 2\kappa u_{2r} + e^* E \end{aligned} \quad (1.7)$$

and,

$$\begin{aligned} m_2 \frac{d^2 u_{2r+1}}{dt^2} &= -m_2 \omega^2 u_{2r+1} = \kappa(u_{2r+2} + u_{2r} - 2u_{2r+1}) - e^* E \\ &= \kappa(e^{-i2qa} + 1)u_{2r+2} - 2\kappa u_{2r+1} - e^* E \end{aligned} \quad (1.8)$$

where, E is the electric field associated due to coulomb effect produced by the charges $\pm e^*$.

Now, in the long wavelength limit, $q \rightarrow 0$, all the particles with same mass are displaced equally along the chain; so, let u_1 and u_2 be the displacement of all particles of m_1 and m_2 respectively

in the long wavelength limit. The force equations (1.7) and (1.8) can be written in the limit $q \rightarrow 0$ as shown below:

$$-(\omega^2 - \omega_0^2)u_1 = \frac{e^*E}{m_1} \quad (1.9)$$

and,

$$-(\omega^2 - \omega_0^2)u_2 = \frac{e^*E}{m_2} \quad (1.10)$$

where, $\omega_0 = 2\kappa \left(\frac{1}{m_1} + \frac{1}{m_2} \right)$ is the square of the resonant frequency in the absence of any charge ($e^* = 0$). Defining the interatomic displacement, $u = u_1 - u_2$, Eq. (1.9) and (1.10) can be written as:

$$(\omega_0^2 - \omega^2)u = e^* \left(\frac{1}{m_1} + \frac{1}{m_2} \right) E \quad (1.11)$$

The Eq. (1.11) clearly shows that the electric field produced is directly proportional to the interatomic displacement.

Now, if N be the total number of atomic pairs per unit volume, then the associated polarization P , which defines the dipole moment per unit volume can be written as:

$$P = \frac{Ne^*u}{\epsilon(\infty)} = \frac{1}{\epsilon(\infty)} \frac{Ne^{*2}}{(\omega_0^2 - \omega^2)} \left(\frac{1}{m_1} + \frac{1}{m_2} \right) E \quad (1.12)$$

Eq. (1.12) is very significant in the sense that it gives the polarization produced due to longitudinal vibrational normal modes (LO phonons) modelled for a diatomic crystal modelled as a 1d linear chain, this forms the basis for electron – phonon interaction, so called Fröhlich interaction to be explained in the later section and it has been used in this thesis (under the purview of dielectric

continuum model) for modelling charge carrier scattering in semiconductor devices and their nanostructures. It should be noted that in the long wavelength limit $q \rightarrow 0$, we see from Eq. (1.8) and (1.9):

$$-m_1 u_1 = m_2 u_2 \quad (1.13)$$

Eq. (1.12) brings forth the fact that the atoms vibrate out-of-phase for the case of optical phonons and it can similarly be shown that for LA phonon they vibrate in-phase.

The preceding paragraphs highlight the importance of LO phonons in the production of macroscopic polarization in semiconductor materials, this polarization field is responsible for exchange of energy with the charge carriers and is the dominant scattering mechanism over wide ranging parameters[1]. On the other hand, Transverse Optical (TO) phonon modes have the particle displacement normal to the wave vector ($\mathbf{q} \cdot \mathbf{P} = 0$) and hence they are not significant for carrier energy exchange, but they are related to dielectric constant of the material through Lydanne-Sachs-Teller relation as shown below:

$$\epsilon(\omega) = \epsilon(\infty) \frac{\omega^2 - \omega_{LO}^2}{\omega^2 - \omega_{TO}^2} \quad (1.14)$$

where, $\epsilon(\omega)$ is the dielectric function of the material, ω_{LO} and ω_{TO} are the characteristic LO and TO phonon frequency of the medium.

Continuing with the motivation of production of polarization field because of vibrational normal modes in a material, Loudon (1964) described the optical phonons in terms of macroscopic

field equations (derived from Maxwell's equation). Briefly, in Loudon's model the general expression relating E and P are:

$$E = \frac{-4\pi[\mathbf{q}(\mathbf{q} \cdot \mathbf{P}) - \omega^2 \mathbf{P}/c^2]}{q^2 - \omega^2/c^2} \quad (1.15)$$

For LO mode, $\mathbf{q} \cdot \mathbf{P} = qP$, which if substituted in Eq. (15) results in:

$$\mathbf{E} = -4\pi\mathbf{P} \quad (1.16)$$

Similarly, for TO mode, substituting $\mathbf{q} \cdot \mathbf{P} = 0$ results in:

$$\mathbf{P} = \frac{1}{4\pi} \left\{ \frac{[\epsilon(0) - \epsilon(\infty)]\omega_{TO}^2}{\omega_{TO}^2 - \omega^2} + [\epsilon(\infty) - 1] \right\} \mathbf{E} \quad (1.17)$$

1.3 Modification of phonon dispersion:

The presence of interfaces (as in the case of transistors), or due to dimensional confinement, the phonon dispersion relation undergoes significant modification.[3] Classifies these modes for the case of single heterostructure for optical phonon modes as follows:

- (a) Interface modes: The modes whose amplitude of vibration shows exponential decay as we move farther from the interface. These modes become very significant for studying near surface carrier transport and also they have been shown to have fast phonon – assisted transitions in quantum well lasers [4].

(b) Half space LO mode: These modes have the frequency same as the bulk LO mode, and they exist in one medium only, the polarization does not exist in the other medium and whose component of polarization field parallel to the interface vanishes.

(c) Half space TO mode: These modes have the frequency same as the bulk TO mode, and they exist in one medium only, the polarization does not exist in the other medium and whose normal component of polarization to the interface vanishes.

Single and double heterostructures of polar cubic crystals have been studied extensively under the purview of dielectric continuum model [1,3-5]; the dispersion relation for a single interface separating two semi-infinite polar mediums with dielectric constants $\epsilon_1(\omega)$ and $\epsilon_2(\omega)$ is given by the solution of the following equation:

$$\epsilon_1(\omega) + \epsilon_2(\omega) = 0 \quad (1.18)$$

The solution of above equation results in two modes namely symmetric (lower frequency) and anti-symmetric mode (higher frequency), these are named according to the symmetry of associated Fröhlich potential about the interface. In ref [6], a transfer matrix method was employed to find a generalized solution to dispersion relation for polar cubic materials having any arbitrary n interface. Such a system will have $2n$ optical phonon modes (two modes: symmetric/anti-symmetric for every interface).

Similarly, for wurtzite heterostructures studies have been conducted in Ref [7-10]. In [10], a generalized expression for dispersion relation for a double heterostructure consisting of a wurtzite material in the middle which is sandwiched by two different materials on left and right was derived along with their associated Fröhlich potential. The generalized dispersion relation for symmetric and anti-symmetric mode is given as:

$$\left(\epsilon_{1z}k_1 + \epsilon_{2z}k_2 \tanh\left(\frac{k_2d}{2}\right) \right) \left(\epsilon_{3z}k_3 + \epsilon_{2z}k_2 \tanh\left(\frac{k_2d}{2}\right) \right) = 0 \quad (1.19)$$

$$\left(\epsilon_{2z}k_2 + \epsilon_{1z}k_1 \tanh\left(\frac{k_2d}{2}\right) \right) \left(\epsilon_{2z}k_2 + \epsilon_{3z}k_3 \tanh\left(\frac{k_2d}{2}\right) \right) = 0 \quad (1.20)$$

For proper treatment of carrier – optical phonon interaction, the modification in optical phonon dispersion should be properly accounted for.

In this thesis, the interface modes for acoustic phonons (quantized Rayleigh waves) in diamond crystal – their description and interaction with charge carriers are treated in-depth in chapter 2, followed by that results of interface mode (IF) solution for optical phonon modes will be applied to a single heterostructure in chapter 3 for cubic Boron Nitride/ Diamond high electron mobility transistor (HEMT). Also, in chapter 9 the dielectric continuum model to evaluate confined optical mode in the context of spherical quantum dot.

1.4 Electron – phonon interaction mechanism

In this thesis the following two interaction mechanisms have been studied:

1. **Fröhlich interaction:** As discussed in section 1.1, the longitudinal optical (LO) modes in polar materials create polarization field, $\mathbf{P}(\mathbf{r})$ which interacts with the charge carriers causing them to gain/lose energy – this interaction is referred to as Fröhlich interaction. At

room temperature, this interaction results in the dominant scattering mechanism for polar semiconductors. The Fröhlich potential, ϕ_{Fr} associated with the polarization field, $\mathbf{P}(\mathbf{r})$ are related as follows:

$$\nabla^2 \phi_{Fr}(\mathbf{r}) = 4\pi \nabla \cdot \mathbf{P}(\mathbf{r}) \quad (1.21)$$

For, a bulk isotropic material consisting of diatomic unit cell with atomic masses m_1 and m_2 and consisting of N atomic dipoles per unit volume, the polarization can be expressed in the second quantized form as follows [1]:

$$\mathbf{P}(\mathbf{r}) = \zeta \sum_{j=1,2,3} \int \frac{d^3 \mathbf{q}}{(2\pi)^3} (a_{\mathbf{q}} e^{i\mathbf{q} \cdot \mathbf{r}} \mathbf{e}_{\mathbf{q},j} + a_{\mathbf{q}}^\dagger e^{-i\mathbf{q} \cdot \mathbf{r}} \mathbf{e}_{\mathbf{q},j}^*) \quad (1.22)$$

where, $a_{\mathbf{q}}$ and $a_{\mathbf{q}}^\dagger$ are the phonon annihilation and creation operator respectively, $\mathbf{e}_{\mathbf{q},j}$ is the polarization vector and ζ is the coupling constant defined as:

$$\zeta = \frac{Ne^*}{\epsilon(\infty)\sqrt{N}} \sqrt{\frac{\hbar}{2\left(\frac{m_1 m_2}{m_1 + m_2}\right)\omega_{LO}}} = \sqrt{\frac{\hbar}{2\omega_{LO}} \cdot \frac{\omega_{LO}^2}{4\pi} \left(\frac{1}{\epsilon(\infty)} - \frac{1}{\epsilon(0)}\right)} \quad (1.23)$$

Now, since the Fröhlich interaction Hamiltonian is defined as: $H_{Fr} = -e\phi_{Fr}$, using Eq (1.21), (1.22) and (1.23) with the fact that $\mathbf{e}_{\mathbf{q},j} \cdot \mathbf{q} = 0$, the final expression of H_{Fr} is given below:

$$H_{Fr} = -i \sqrt{\frac{2\pi e^2 \hbar \omega_{LO}}{V} \left(\frac{1}{\epsilon(\infty)} - \frac{1}{\epsilon(0)}\right)} \sum_{\mathbf{q}} \frac{1}{q} (a_{\mathbf{q}} e^{i\mathbf{q} \cdot \mathbf{r}} + a_{\mathbf{q}}^\dagger e^{-i\mathbf{q} \cdot \mathbf{r}}) \quad (1.24)$$

where, V is the volume of the material. The $\frac{1}{q}$ dependence arises due to coulombic effect.

2. Deformation potential interaction:

The acoustic phonons interact with the charge carriers with the deformation potential mechanism introduced by Bardeen and Shockley. The atomic displacement associated with the acoustic phonon mode produce strain in the material which changes the lattice constant locally and hence causes change in the local deformation of energy bands. Also, since the kinetic energy of the carrier depends on the location of energy state with respect to band edge, thus, a change in band structure would affect the kinetic energy of the carrier. The local change in energy band for a material with lattice const a is given by:

$$E_{c,v}(a) = \frac{dE_{c,v}(a)}{dV} \Delta V \quad (1.24)$$

where, V is the volume of the element and ΔV represents change in the volume. For and isotropic material, using $\frac{\Delta V}{V} = \nabla \cdot \mathbf{u}$, where u is the displacement of the atom, also, the c, v in the subscript indicates the conduction and valence band respectively. We can define interaction Hamiltonian as the energy associated with the local deformation defined by Eq. (24):

$$H_{def}^{c,v} = \Delta E_{c,v}(a) = E_1^{c,v} \nabla \cdot \mathbf{u} \quad (1.25)$$

where, $E_1^{c,v}$ is the deformation potential (which is different for electrons and holes).

1.5 Emerging Semiconductors

Historically, Silicon has been the main driver of the semiconductor revolution, however, its application to high power and high frequency applications such as electric aerospace, automotives and grid infrastructure is limited due to its narrow band gap 1.12 eV (indirect), low

thermal conductivity (~ 1.5 W/cm-K) , low break down field (~ 300 KV/cm) and limited room temperature mobility ($\sim 1.5 \times 10^3 \frac{cm^2}{V-sec}$ for electrons) [11]. On the other hand, the wide band gap semiconductors namely SiC (3.03 eV for 6H and 3.26 eV for 4H) and GaN (3.45 eV) have higher breakdown field (2500 KV/cm for 6H , 2200 KV/cm for 4H SiC and 2000 KV/cm for GaN), higher thermal conductivity (4.9 W/cm-K for SiC) and superior reliability which make them more suitable for high power and high frequency applications.

The III- nitrides (typically GaN and its alloys with Al and In) have a direct bandgap which are tunable in the range of 6.4 eV (AlN) to 3.4 eV (GaN) to 0.7 eV (AlN) which covers the range from deep ultra violet to infra red range thus finding wide application in LEDs, laser diodes, solar cells and many optoelectronic applications [12,13] . Also, for RF applications the High Electron Mobility transistor based on two dimensional electron gas (2DEG) at AlGaIn/GaN interface shows a mobility in the range $1200 - 2000 \frac{cm^2}{V-sec}$ with a power capability of 40 W/mm [13]. These III-nitrides and SiC generally crystalize in wurtzite phase at room temperature.

Similarly, II -VI semiconductors such as CdS, CdSe, ZnO and ZnS are other promising candidates in optoelectronics, HEMT and SAW devices [14]. Finally, Diamond with a bandgap of ~ 5.5 eV is emerging as a potential candidate for high frequency FET and high power switching applications [13,15]. Its high bulk room temperature electron mobility $4500 \frac{cm^2}{V-sec}$ and hole mobility of $3800 \frac{cm^2}{V-sec}$ is making it possible for high frequency applications. Also, it has a very high value of thermal conductivity 22 W/cm-K and breakdown field strength greater than 10MV cm^{-1} makes it very attractive for high power switches [15].

In this thesis an effort is made to investigate phonon interactions with charge carriers in the above materials to study carrier transport and also, to understand acoustic phonon decay in wurtzite crystals using 2H-SiC material as an example to understand the thermal conductivity in general.

1.6 Organization of thesis

The research work presented in this thesis is organized as follows: Chapter 2, Investigation on the effects of surface-acoustic phonon scattering on the charge transport behavior of diamond based FET devices. Motivated by the promising role of diamond in the realization of high power and high frequency electronic devices, this work is focus on detailed formulation of relaxation times due to the hole-surface-acoustic phonon scattering, which appears to have been an overlooked scattering mechanism important to diamond-based devices. The matrix element, scattering rates and relaxation times have been calculated by taking into account, for the first time Rayleigh waves near the surface. This is achieved by quantizing the Rayleigh waves and using the corresponding acoustic phonon to calculate the Fermi golden rule based scattering rate of holes in the two-dimensional hole gas. The results show that the scattering of holes with surface acoustic Rayleigh waves reduced relative to scattering from bulk 3D acoustic phonons. Moreover, the mobilities are found to be higher than those based on the theory for 3D acoustic phonons. The results reveal significant insights to diamond based electronics having acoustic phonons Rayleigh waves thus opening new research endeavors.

In Chapter 3 the investigation of phonon-dominated mobilities for carriers in a diamond field effect transistor with a cubic Boron Nitride (cBN) overlayer is done. This chapter investigates specifically, the intra-subband scattering due to interaction of electrons with acoustic phonons,

treated properly as quantized surface acoustic Rayleigh waves, and inclusion, for the first time, the interaction with remote polar phonons originating in the cBN overlayer. It is concluded that the surface acoustic phonon scattering is the dominant mechanism limiting the mobility of electrons for temperatures below 375 K.

In Chapter 4 a systematic study of acoustic phonon decay mechanism is done for wurtzite crystals in general by taking 2H-SiC polytype as an example. Due to the presence of elastic anharmonicity, it is predicted that the longitudinal acoustic (LA) phonons in 2H-SiC will exhibit decay paths to lower-order modes through two key decay processes. Specific investigation of spontaneous decay of LA phonons in the quasi-isotropic 2H-SiC wurtzite crystal taking the spatial anisotropy into account has been done. It is shown that in the plane containing the c-axis the decay rate for the process $LA \rightarrow LA + TA$ (Transverse acoustic) dominates, whereas, for the plane normal to the c-axis (the XY plane) $LA \rightarrow TA+TA$ dominates. The overall scattering rate in XY plane is higher than the plane containing the c-axis.

As discussed in Chapter 5, it is well known that the carrier—optical-phonon scattering rates dominate the carrier—acoustic-phonon scattering rates in many polar materials of interest in electronic and optoelectronic applications. Furthermore, it is known that the Fröhlich coupling constants for carrier-optical-phonon in many materials is close to or great than unity, calling into question the validity of scattering rates based on the Fermi golden rule. In a celebrated paper by Thornber and Feynman it was shown that that the large Fröhlich coupling constant in polar materials does indeed lead to substantial corrections to the Fermi golden rule scattering rates. These large corrections are due to the fact that for strong coupling constants, the first-order perturbative approach underlying the Fermi golden rule does not take into account the presence of

many phonons interacting simultaneously with the carrier. In this paper, the Thorner-Feynman scattering rates for carrier—optical-phonon interactions are derived for several technologically important wurtzite semiconductors – BN, ZnO, CdS, CdSe, ZnS, InN, and SiC – and it is shown that the commonly used Fermi’s golden rule scattering rates must be corrected by factors ranging up to an order-of-magnitude. The corrections to the Fermi’s golden rule reported herein have widespread impact on carrier transport for materials with large Fröhlich coupling constants.

Chapter 6 deals with III-Nitride semiconductors with cubic crystal structure have shown promise for enhanced efficiency in photonic and optoelectronic applications. The recent interest in cubic III-Nitrides has arisen due to the inability to realize enhanced efficiency in optoelectronic applications of the wurtzite phase due to spontaneous polarization effects, crystal defects due to growth on lattice mismatched substrates and also for requirement of fabricating normally off transistors for high mobility transistors. The cubic III-Nitride materials are characterized by strong coupling of carriers to optical phonons in which the standard perturbative approach – based on first order perturbation theory – breaks down. In this chapter, the necessary corrections to Fermi’s-golden-rule electron – optical phonon matrix elements for selected cubic III-Nitrides via the non-perturbative Thorner – Feynman path-integral techniques has been determined. Specifically, the electron transport parameters such as the threshold electric field, threshold velocity, mobility and runaway length for BN, AlN, GaN and InN has been reported.

Chapter 7 considers the evaluation of the electric field – velocity relation for strong electron – LO phonon coupled 2D materials namely HfS_2 , $HfSe_2$, ZrS_2 and $ZrSe_2$ by applying Thorner – Feynman (TF) formalism applied to the case of the 2D Fröhlich polaron. It is further demonstrated that the generally-accepted Fermi’s Golden Rule based approach breaks down for

these strongly coupled materials. It is further predicted that $ZrSe_2$ has highest mobility of $449.1 \text{ cm}^2/V\text{-s}$ at room temperature followed by $HfSe_2$ with $239.78 \text{ cm}^2/V\text{-s}$ whereas other materials have below $100 \text{ cm}^2/V\text{-s}$.

In Chapter 8 the role of confined longitudinal optical (LO) phonons is investigated under the purview of dielectric continuum model in creation of excitons in a strongly confined GaAs quantum dot. It is found that at low temperatures (below 10 K) the confined LO mode exciton creation rate is 6.87 times (~ 7 times) slower as compared to bulk acoustic phonons for exciton occupancy of 80% and above. Though acoustic phonons dominate the exciton creation, the role of confined LO phonons cannot be neglected, hence this work provides a basis for confined LO phonon assisted exciton creation in self assembled spherical quantum dots.

Chapter 2

SURFACE-ACOUSTICS PHONON SCATTERING IN 2D-HOLE GAS OF DIAMOND BASED FET DEVICES

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2.1 Introduction

Recently, the demand for devices that can operate in harsh conditions such as high temperature, high power or high frequency has been increased significantly. Silicon, a traditional industry material is not suitable for such purposes because of its narrow band gap. As an alternative, wide band gap semiconductor materials have been explored [16]. In particular, diamond has evolved as a promising material due to its exceptional physical properties such as intrinsically high break down field (>10 MV/cm) [17], wide bandgap (5.46 – 5.6 eV) [18] and high thermal conductivity [19]. One of the most outstanding diamond properties includes its high carrier mobility and particularly for holes in comparison with its neighboring semiconductors such as Si or SiC [20]. Progress in the development of diamond based electronic devices has been made on a number of fronts ([IEEE TED, Vol 67, No 6, June 2020, PP-2270-2275], Crawford *et al.*; Pernot *et al.*; Zhang *et al.*) [21]- [23]. So far most of the efforts that have been directed at understanding the factors affecting conductivity are associated with external doping such as using surface acceptor oxide layers or scattering in bulk materials only [24]. Another most important factor in the mobility of diamond is the scattering mechanisms resulting from the two dimensional hole gas (2DHG) instead of bulk material which is induced at the surface of hydrogen terminated (H-terminated) diamond. There have been very few reports to date that present a detailed quantitative

description of scattering mechanisms responsible for mobility limitation in 2DHG of diamond devices.

When diamond is terminated by hydrogen, it induces a negative electron affinity along with high room-temperature p-type surface conductivity [25]- [26]. Five scattering mechanisms that play a key role in the mobility of 2DHG in H-terminated diamond include: (1) surface impurity scattering; (2) non-polar optical phonon scattering; (3) surface roughness scattering; (4) acoustic phonon scattering and (5) interface phonon scattering [12]. In our previous study, Bonomo *et al.* presented in detail the role of remote interface polar phonon modes on the electronic transport properties of diamond structures [28]. Our work laid a milestone for understanding interface phonons that penetrate to the two-dimensional hole gas (2DHG) in confined diamond structures. With the exception of Bonomo *et al.* work, past studies of phonon-hole interactions in diamond-based electronic devices have been modeled based by considering only bulk phonons. There is now a growing understanding of carrier-phonon interactions for confined and interface phonon modes as well as applications of phonon engineering in electronic and optoelectronic devices (Stroscio *et al.* ; Komirenko *et al.* ; Park *et al.*,) [1, 29, 30]. In this work, we have modeled the interaction of acoustic phonons with the 2DHG by properly taking into account the fact that the acoustic phonons in the vicinity of the 2DHG are Rayleigh waves and not bulk acoustic waves. We find substantially smaller scattering rates for the case of the Rayleigh wave interface phonons than for bulk phonons.

Considering the lattice vibrations in nanostructures, principle phenomena that alter the process of scattering include the following: firstly, reduction of hole momentum space dimensionality that originates interesting properties related to the hole-phonon interaction kinematics, secondly modifications of the phonon modes caused by the dielectric and acoustic mismatches in the nanostructure materials causes changes in properties of these materials [1]. Thus

for the design of diamond based FETs, effects from surface acoustic phonon limited mobility and the screening of free carriers are of high relevance. In this work, we present a model to theoretically understand carrier transport mechanism due to surface acoustic phonon scattering in diamond based devices. The acoustic phonon scattering mechanism has been investigated using deformation-potential theory, matrix element calculations, scattering rates and taking into account the Rayleigh waves near the surface for the first time.

The paper is organized as follows: In Section II, we explain the existence of Rayleigh waves under consideration in diamond structures for surface acoustic wave analysis. Section III describe the peculiarities of the acoustic-phonon modes and its quantization. Section IV addresses the analytical expressions for the matrix elements of the hole-phonon interaction and deformation potential while Section V presents the conclusions.

2.2 Rayleigh Surface Waves Existence

The surface acoustic wave relevant for this system is the Rayleigh wave. Considering the general case for Lamb waves, if the shear velocity (V_s') in the plate and shear velocity (V_s) in the substrate differs significantly ($V_s' \gg V_s$), a generalized single Lamb wave solution exists that reduces to Rayleigh wave in the system (for which $\beta H \rightarrow 0$) where β is the wave propagation constant and H as the thickness of the elastic plate over diamond structure. For ($V_s' \ll V_s$), an infinite number of solutions exists, that are divided into M_1 and M_2 series families of modes. When H (plate thickness) tends to zero, M_{11} mode tends to a Rayleigh surface wave in the substrate whereas higher M_1 and all M_2 modes appear to be leaky waves [31]. When $\beta H \rightarrow \infty$, all modes from M_{21} and above tend to be the shear velocity (V_s') of the plate while for $\beta H \rightarrow 0$, only the Rayleigh waves exist in the substrate (M_{11}); thus, Rayleigh waves in diamond structures are going to be analyzed solely.

2.3 Acoustic Phonon Quantization Model

In this model, we have investigated scattering rates for holes in the 2-dimensional hole gas (2DHG) with surface acoustic waves for a diamond-based field effect transistor (FET). The 2DHG wave function is taken to be the Fang-Howard variational function. In this regard, the initial hole state obeys the equation as:

$$\Psi_i(r) = \langle r|k \rangle = \sqrt{\frac{b^3}{2}} (y-l) e^{-\frac{1}{2}b(y-l)} \frac{e^{ik_{\parallel}r_{\parallel}}}{\sqrt{S}} \quad (2.1)$$

While the final hole state is defined as,

$$\Psi_f(r) = \langle k'|r \rangle = \sqrt{\frac{b^3}{2}} (y-l) e^{-\frac{1}{2}b(y-l)} \frac{e^{-ik'_{\parallel}r_{\parallel}}}{\sqrt{S}} \quad (2.2)$$

Thus, the probability density function is given as below:

$$\begin{aligned} |\Psi_i(r)|^2 &= \int_{y=l}^{\infty} \int_{z=0}^{z=Z} \int_{x=0}^{x=X} dx dz dy \left| \sqrt{\frac{b^3}{2}} (y-l) e^{-\frac{1}{2}b(y-l)} \frac{e^{-ik_{\parallel}r_{\parallel}} + e^{ik_{\parallel}r_{\parallel}}}{\sqrt{S}} \right|^2 \\ &= \int_l^{\infty} dy \left(\sqrt{\frac{b^3}{2}} \right)^2 (y-l)^2 e^{-b(y-l)} \end{aligned} \quad (2.3)$$

where $\parallel$ direction corresponds to x- z plane (we will drop the $\parallel$ subscript in the following sections),

b is a variational parameter such that $b = \left(\frac{33m^*e_h^2N_h}{8\epsilon_0\epsilon_r\hbar^2} \right)^{\frac{1}{3}}$ [32] and $N_h = 1.8 \times 10^{17} \text{ m}^{-2}$, [33]. S

represents the area of substrate in x-z plane and l represents the depth below the surface at which the infinite barrier of triangular potential well is located which in our case is the diamond surface, hence $l = 0$ in the present case. It is to be noted that the upper limit of y has been taken to infinity because the area under the curve evaluates to 99.99% for a depth of $l + 3 \text{ nm}$, hence for all practical thickness of substrates greater than $l + 3 \text{ nm}$ it does not affect if the upper limit is taken to infinity. The probability density function is plotted in Fig. 1; it is observed that the function peaks at a depth of 660 pm which can be taken as the depth at which 2DHG is located.

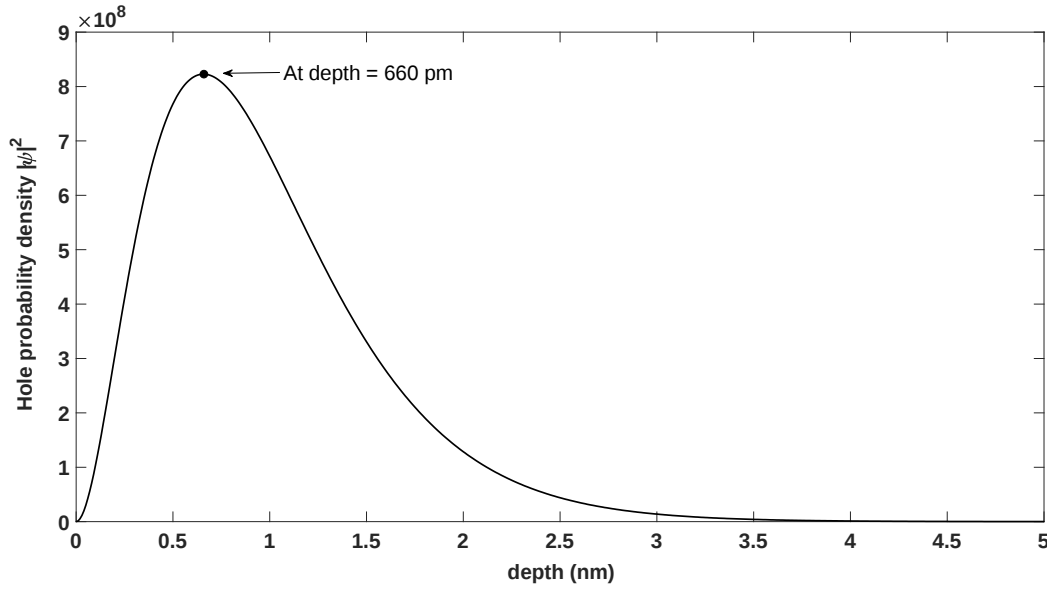


Fig. 2.1 Fang-Howard Probability density function for hole in 2DHG in diamond showing peak at 660 pm.

Herein, the particle displacement expression for classical Rayleigh waves is second quantized so the matrix element of the Rayleigh wave with the hole wavefunctions corresponds to the emission or absorption of a single phonon. The Rayleigh wave amplitude has been studied extensively and the basic elements are described by Graff *et al.* [34] for Rayleigh waves, it is possible to formulate

the displacement of the particles for a wave traveling to the right on an isotropic substrate along the z axis:

$$u_y = -A(\alpha_{tl}e^{-\alpha_{tl}y} - 2\frac{\alpha_{tl}\beta_R^2}{\beta_R^2 + \alpha_{ts}^2}e^{-\alpha_{ts}y})e^{i(\beta_R z - \omega t)} \quad (2.4)$$

And,

$$u_z = iA\beta_R(e^{-\alpha_{tl}y} - 2\frac{\alpha_{ts}\alpha_{tl}}{\beta_R^2 + \alpha_{ts}^2}e^{-\alpha_{ts}y})e^{i(\beta_R z - \omega t)} \quad (2.5)$$

where β_R , α_{tl} and α_{ts} represents the Rayleigh wave propagation constants respectively and the imaginary parts of the transverse wave vector components for the longitudinal and shear partial waves respectively.

For these Raleigh waves, we can write the expressions as:

$$\beta_R^2 - \alpha_{tl}^2 = \left(\frac{\omega}{V_l}\right)^2 \quad (2.6.1)$$

And,
$$\beta_R^2 - \alpha_{ts}^2 = \left(\frac{\omega}{V_s}\right)^2 \quad (2.6.2)$$

And,
$$V_R = \frac{\omega}{\beta_R} \quad (2.6.3)$$

where V_R , V_l and V_s are the Rayleigh wave, longitudinal wave and shear wave velocities, respectively.

The dispersion relation for these Rayleigh waves is given by;

$$4\beta_R^2\alpha_{ts}\alpha_{tl} = (\alpha_{ts}^2 - \beta_R^2)^2 \quad (2.7)$$

which can be approximated as presented by Auld *et al.* [17]

$$\frac{V_R}{V_s} = \frac{0.87 + 1.12\sigma}{1 + \sigma} \quad (2.8)$$

where σ is the material's Poisson ratio.

From well known standard elastic theory relations, we may recall as:

$$V_s = \sqrt{\frac{\mu}{\rho}} \quad (2.9.1)$$

$$\text{And,} \quad V_l = \sqrt{\frac{\lambda + 2\mu}{\rho}} \quad (2.9.2)$$

$$\text{And,} \quad \sigma = \frac{1 - 2 (V_s/V_l)^2}{2[1 - 2 (V_s/V_l)^2]} \quad (2.9.3)$$

where ρ is the density of diamond and λ and μ are the first and second Lamé parameters for diamond.

Introducing the displacement vector which is known to be of the form:

$$u(x, y, z) = \nabla\Phi + \nabla \times \psi \quad (2.10)$$

where Φ and ψ satisfy,

$$\nabla^2\Phi - \frac{1}{V_l^2} \frac{\partial^2\Phi}{\partial t^2} = 0 \quad (2.11.1)$$

$$\nabla^2\psi - \frac{1}{V_s^2} \frac{\partial^2\psi}{\partial t^2} = 0 \quad (2.11.2)$$

and it follows that,

$$\Phi = Ae^{-\alpha_{tl}y} e^{i(\beta_{RZ}-\omega t)} = \phi(y) e^{i(\beta_{RZ}-\omega t)} \quad (2.11.3)$$

$$\psi = A \left(-\frac{2i\alpha_{tl}\beta_R}{\alpha_{ts}^2 + \beta_R^2} \right) e^{-\alpha_{ts}y} e^{i(\beta_R z - \omega t)} = \psi(y) e^{i(\beta_R z - \omega t)} \quad (3.11.4)$$

Thus the Rayleigh wave phonon may be quantized as outlined in Strocio and Dutta [1] using the condition,

$$\frac{1}{cL} \int_0^c dz \int_0^{+\infty} u(\beta_R, y, z) \cdot u^*(\beta_R, y, z) dy = 1 \quad (2.12)$$

where c and L are the normalization lengths along the horizontal and vertical axis of the diamond film respectively. Further ω_{β_R} is considered to be the angular frequency of the mode with wave vector as β_R .

The quantities,

$$\begin{aligned} u_y \cdot u_y^* &= A^2 \alpha_{tl}^2 \left(e^{-\alpha_{tl}y} - 2 \frac{\beta_R^2}{\beta_R^2 + \alpha_{ts}^2} e^{-\alpha_{ts}y} \right)^2 \\ &= A^2 \alpha_{tl}^2 \left(e^{-2\alpha_{tl}y} - 4 \frac{\beta_R^2}{\beta_R^2 + \alpha_{ts}^2} e^{-(\alpha_{tl} + \alpha_{ts})y} + 4 \frac{\beta_R^4}{(\beta_R^2 + \alpha_{ts}^2)^2} e^{-2\alpha_{ts}y} \right) \end{aligned} \quad (2.13)$$

and

$$\begin{aligned} u_z \cdot u_z^* &= A^2 \beta_R^2 \left(e^{-\alpha_{tl}y} - 2 \frac{\alpha_{ts}\alpha_{tl}}{\beta_R^2 + \alpha_{ts}^2} e^{-\alpha_{ts}y} \right)^2 \\ &= A^2 \beta_R^2 \left(e^{-2\alpha_{tl}y} - 4 \frac{\alpha_{ts}\alpha_{tl}}{\beta_R^2 + \alpha_{ts}^2} e^{-(\alpha_{ts} + \alpha_{tl})y} + 4 \frac{4\alpha_{ts}^2\alpha_{tl}^2}{(\beta_R^2 + \alpha_{ts}^2)^2} e^{-2\alpha_{ts}y} \right) \end{aligned} \quad (2.14)$$

are needed to define the integrand of the normalization condition and to obtain,

$$\begin{aligned}
& \frac{1}{L} \int_0^\infty A^2 \alpha_{tl}^2 (e^{-2\alpha_{tl}y} - 4 \frac{\beta_R^2}{\beta_R^2 + \alpha_{ts}^2} e^{-(\alpha_{tl} + \alpha_{ts})y} \\
& \quad + 4 \frac{\beta_R^4}{(\beta_R^2 + \alpha_{ts}^2)^2} e^{-2\alpha_{ts}y}) dy \\
& \quad + \frac{1}{L} \int_0^\infty A^2 \beta_R^2 (e^{-2\alpha_{tl}y} - 4 \frac{\alpha_{ts}\alpha_{tl}}{\beta_R^2 + \alpha_{ts}^2} e^{-(\alpha_{ts} + \alpha_{tl})y} \\
& \quad + \frac{4\alpha_{ts}^2\alpha_{tl}^2}{(\beta_R^2 + \alpha_{ts}^2)^2} e^{-2\alpha_{ts}y}) dy = 1
\end{aligned} \tag{2.15}$$

Accordingly,

$$\begin{aligned}
& \frac{A^2 \alpha_{tl}^2}{L} \left[\frac{e^{-2\alpha_{tl}y}}{-2\alpha_{tl}} \Big|_0^{+\infty} - 4 \frac{\beta_R^2}{\beta_R^2 + \alpha_{ts}^2} \frac{e^{-(\alpha_{tl} + \alpha_{ts})y}}{-(\alpha_{tl} + \alpha_{ts})} \Big|_0^{+\infty} + 4 \frac{\beta_R^4}{(\beta_R^2 + \alpha_{ts}^2)^2} \frac{e^{-2\alpha_{ts}y}}{-2\alpha_{ts}} \Big|_0^{+\infty} \right] + \\
& \frac{A^2 \beta_R^2}{L} \left[\frac{e^{-2\alpha_{tl}y}}{-2\alpha_{tl}} \Big|_0^{+\infty} - 4 \frac{\alpha_{ts}\alpha_{tl}}{\beta_R^2 + \alpha_{ts}^2} \frac{e^{-(\alpha_{ts} + \alpha_{tl})y}}{-(\alpha_{ts} + \alpha_{tl})} \Big|_0^{+\infty} + 4 \frac{\alpha_{ts}^2\alpha_{tl}^2}{(\beta_R^2 + \alpha_{ts}^2)^2} \frac{e^{-2\alpha_{ts}y}}{-2\alpha_{ts}} \Big|_0^{+\infty} \right] = 1
\end{aligned}$$

which simplifies as:

$$\begin{aligned}
& \frac{A^2 \alpha_{tl}^2}{L} \left[\frac{1}{2\alpha_{tl}} - \frac{4\beta_R^2}{\beta_R^2 + \alpha_{ts}^2} \frac{1}{\alpha_{tl} + \alpha_{ts}} + \frac{4\beta_R^4}{(\beta_R^2 + \alpha_{ts}^2)^2} \frac{1}{2\alpha_{ts}} \right] \\
& \quad + \frac{A^2 \beta_R^2}{L} \left[\frac{1}{2\alpha_{tl}} - \frac{4\alpha_{ts}\alpha_{tl}}{\beta_R^2 + \alpha_{ts}^2} \frac{1}{\alpha_{tl} + \alpha_{ts}} \right. \\
& \quad \left. + \frac{4\alpha_{ts}^2\alpha_{tl}^2}{(\beta_R^2 + \alpha_{ts}^2)^2} \frac{1}{2\alpha_{ts}} \right] = 1
\end{aligned} \tag{2.16}$$

which may be simplified to,

$$A^2 \left[\frac{\alpha_{tl}}{2} - \frac{4\beta_R^2 \alpha_{tl}^2}{(\beta_R^2 + \alpha_{ts}^2)(\alpha_{tl} + \alpha_{ts})} + \frac{2\beta_R^4 \alpha_{tl}^2}{\alpha_{tl}(\beta_R^2 + \alpha_{ts}^2)^2} + \frac{\beta_R^2}{2\alpha_{tl}} \right] + \left[\frac{\beta_R^2}{2\alpha_{tl}} - \frac{4\alpha_{ts}\alpha_{tl}\beta_R^2}{(\beta_R^2 + \alpha_{ts}^2)(\alpha_{tl} + \alpha_{ts})} + \frac{2\beta_R^2 \alpha_{ts}^2 \alpha_{tl}^2}{(\beta_R^2 + \alpha_{ts}^2)^2} \right] = 1 \quad (2.17)$$

Using the previously defined relations between the wave velocities and β_R , this last result may be simplified to,

$$A^2 \left[\frac{\alpha_{tl}}{2} - \frac{(\beta_R^2 + \alpha_{ts}^2)\alpha_{tl}}{\alpha_{ts}(\alpha_{tl} + \alpha_{ts})} + \frac{2\beta_R^2 \alpha_{tl}}{4\alpha_{ts}^2} + \frac{\beta_R^2}{2\alpha_{tl}} - \frac{(\beta_R^2 + \alpha_{ts}^2)}{(\alpha_{tl} + \alpha_{ts})} + \frac{\alpha_{tl}}{2} \right] = 1 \quad (2.18)$$

and it follows that,

$$A^2 \left[\frac{2\alpha_{ts}^2 \alpha_{tl}^2 (\alpha_{tl} + \alpha_{ts})}{2\alpha_{ts}^2 \alpha_{tl} (\alpha_{tl} + \alpha_{ts})} - \frac{2(\beta_R^2 + \alpha_{ts}^2) \alpha_{tl}^2 \alpha_{ts}}{2\alpha_{ts}^2 \alpha_{tl} (\alpha_{tl} + \alpha_{ts})} + \frac{\beta_R^2 \alpha_{tl}^2 (\alpha_{tl} + \alpha_{ts})}{2\alpha_{ts}^2 \alpha_{tl} (\alpha_{tl} + \alpha_{ts})} + \frac{\beta_R^2 \alpha_{tl}^2 (\alpha_{tl} + \alpha_{ts})}{2\alpha_{ts}^2 \alpha_{tl} (\alpha_{tl} + \alpha_{ts})} - \frac{2\alpha_{ts}^2 \alpha_{tl} (\beta_R^2 + \alpha_{ts}^2)}{2\alpha_{ts}^2 \alpha_{tl} (\alpha_{tl} + \alpha_{ts})} \right] = 1 \quad (2.19)$$

or equivalently,

$$A^2 \left[\frac{2\alpha_{ts}^2 \alpha_{tl}^2}{2\alpha_{ts}^2 \alpha_{tl}} - \frac{2(\beta_R^2 + \alpha_{ts}^2) \alpha_{tl} \alpha_{ts}}{2\alpha_{ts}^2 \alpha_{tl}} + \frac{\beta_R^2 \alpha_{tl}^2}{2\alpha_{ts}^2 \alpha_{tl}} + \frac{\beta_R^2 \alpha_{tl}^2}{2\alpha_{ts}^2 \alpha_{tl}} \right] = 1 \quad (2.20)$$

which implies that the phonon normalization factor is,

$$A = \sqrt{\frac{2\alpha_{ts}^2 \alpha_{tl}}{\beta_R^2 (\alpha_{tl} - \alpha_{ts})^2 + 2\alpha_{ts}^2 \alpha_{tl} (\alpha_{tl} - \alpha_{ts})}} \quad (2.21)$$

2.4 Rayleigh wave displacement pattern

Recalling the displacement expressions from eq. 2.4 & 2.5, and noting that the displacements are real quantities, only spatial component of displacement are taken into consideration thus expressed as below:

$$u_y = Re(u_y) = -A \left(\alpha_{tl} e^{-\alpha_{tl}y} - \frac{2\alpha_{tl}\beta_R^2}{\beta_R^2 + \alpha_{ts}^2} e^{-\alpha_{ts}y} \right) \cos(\beta_R z) \quad (2.22)$$

And,

$$u_z = Re(u_z) = A\beta_R \left(e^{-\alpha_{tl}y} - \frac{2\alpha_{tl}\alpha_{ts}}{\beta_R^2 + \alpha_{ts}^2} e^{-\alpha_{ts}y} \right) \sin(\beta_R z) \quad (2.23)$$

where S is area in x - z plane that is 1 nm^2 . Now, since we know that $\cos^2(\beta_R z) + \sin^2(\beta_R z) = 1$, substituting for $\cos(\beta_R z)$ and $\sin(\beta_R z)$, from eq. 2.1 and 2.2 as:

$$\frac{u_z^2}{A^2 \beta_R^2 \left(e^{-\alpha_{tl}y} - \frac{2\alpha_{tl}\alpha_{ts}}{\beta_R^2 + \alpha_{ts}^2} e^{-\alpha_{ts}y} \right)^2} + \frac{u_y^2}{A^2 \left(\alpha_{tl} e^{-\alpha_{tl}y} - \frac{2\alpha_{tl}\beta_R^2}{\beta_R^2 + \alpha_{ts}^2} e^{-\alpha_{ts}y} \right)^2} = 1 \quad (2.24)$$

The above equation represents an ellipse in y - z plane. However, for different values of y (which represents depth inside the surface) we get a family of ellipses with coordinates of center $\equiv (y, 0)$.

The other properties of ellipse are shown below:

Major axis: along y -axis, length of major axis: $2 A \left(\alpha_{tl} e^{-\alpha_{tl}y} - \frac{2\alpha_{tl}\beta_R^2}{\beta_R^2 + \alpha_{ts}^2} e^{-\alpha_{ts}y} \right)$;

Coordinates of foci: $(y + c, 0)$ and $(y - c, 0)$, where expression of c is given below:

$$c = A \sqrt{\beta_R^2 \left(e^{-\alpha_{tl}y} - \frac{2\alpha_{tl}\alpha_{ts}}{\beta_R^2 + \alpha_{ts}^2} e^{-\alpha_{ts}y} \right)^2 - \left(\alpha_{tl} e^{-\alpha_{tl}y} - \frac{2\alpha_{tl}\beta_R^2}{\beta_R^2 + \alpha_{ts}^2} e^{-\alpha_{ts}y} \right)^2} \quad (2.25)$$

In the context of diamond we observe that u_y undergoes a phase shift by π at depth of $\frac{\lambda_R}{4}$; hence, the elliptically polarized displacement pattern undergoes change in sense of rotation from

anticlockwise to clockwise at depth of $\frac{\lambda_R}{4}$. Further, for depth less than $\frac{\lambda_R}{4}$ since the sense of rotation is anti-clockwise for direction of propagation along positive z-direction; thus, we say that such elliptical motion is retrograde in nature. Fig. 2.2 represents the normalized Y and Z component of Rayleigh wave displacement vectors for $\lambda_R = 500 \text{ pm}$ where as displacements patterns at various depths below the surface are presented in Fig. 2.3.

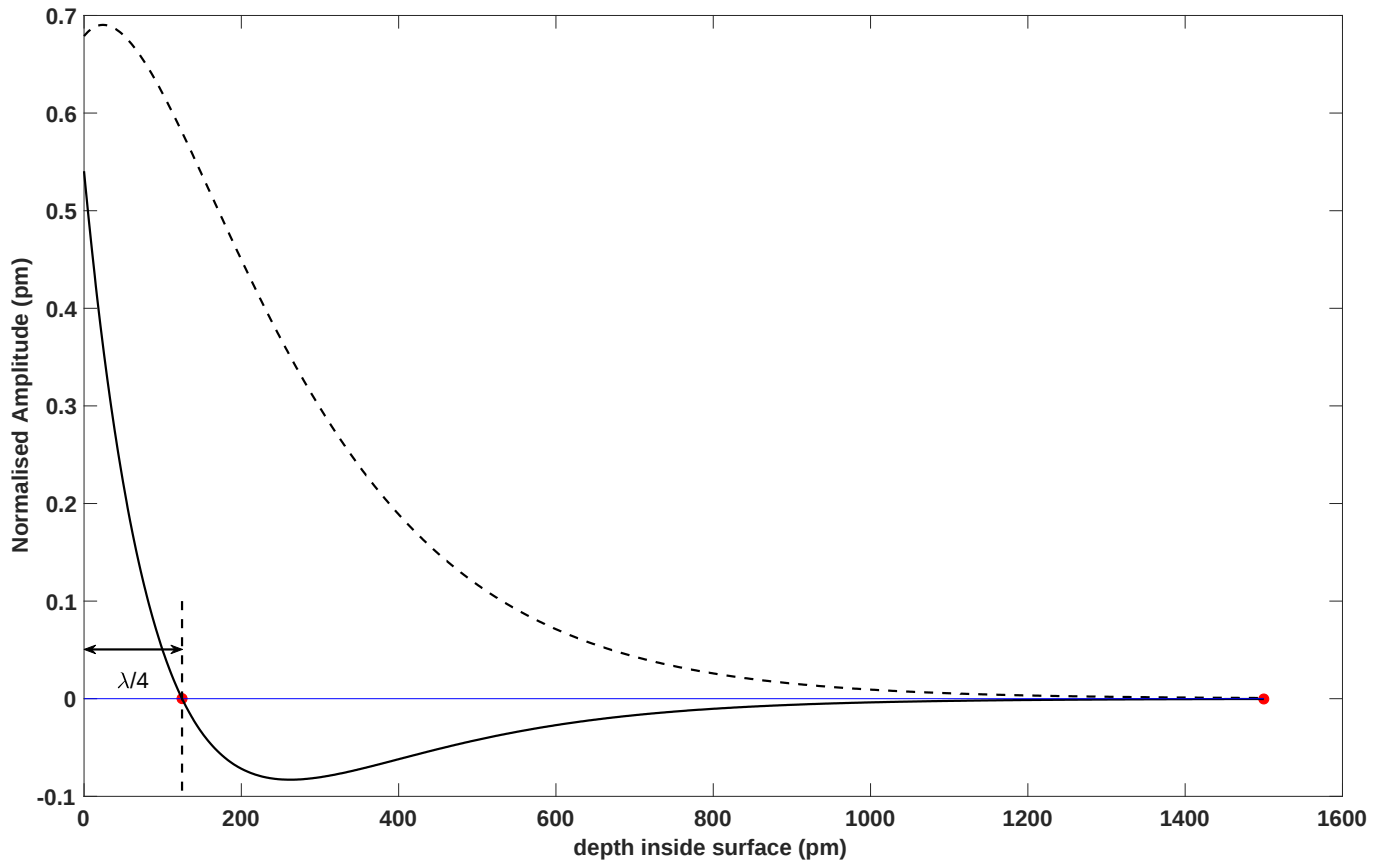


Fig. 2.2 Normalized Y and Z component of Rayleigh wave displacement vectors for $\lambda_R = 500 \text{ pm}$. The dashed line represents the Z component and solid line represents y-component. The y-component changes sign at $y = 124.6 \text{ pm} \approx \frac{\lambda_R}{4}$, it is at this point the sense of rotation changes. The elliptically polarized pattern becomes progressive from retrograde.

Figure 2.2 depicts the normalized Y and Z component of Rayleigh wave displacement vectors for $\lambda_R = 500$ pm. The dashed line represents the Z component and solid line represents the y-component. The y-component changes sign at $y = 124.6$ pm $\approx \frac{\lambda_R}{4}$, it is at this point the sense of rotation changes. The elliptically polarized displacement pattern becomes progressive from retrograde. The change of the sign of the y-component of displacement $\approx \frac{\lambda_R}{4}$ indicates that the ellipse representing the displacement transitions from anti-clockwise to clockwise as a function of depth. This behavior and the depth dependence of the Fang-Howard dependence on N_h – see Eq. 2.3 and the associated discussion – indicate that Rayleigh waves open a new avenue for tuning the mobility as a function of N_h due to the depth variation of the Rayleigh wave displacement pattern which is absent for bulk phonons.

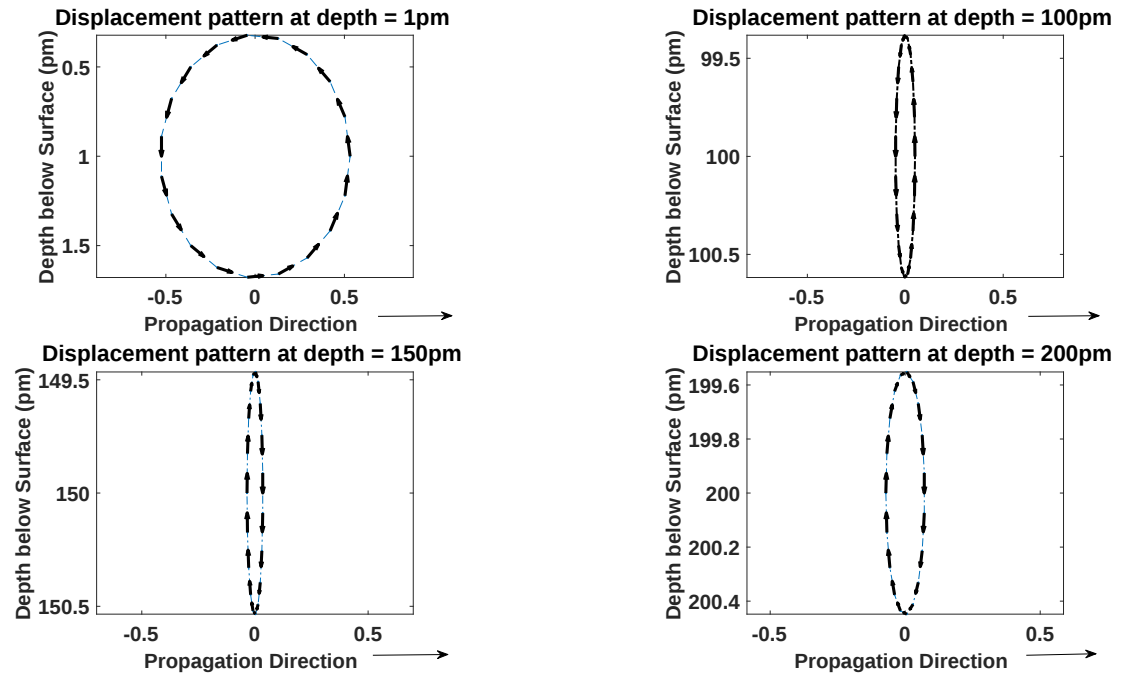


Fig. 2.3 Rayleigh wave displacement pattern plotted at $y = 1, 100, 150$ and 200 pm depth below surface, showing change of sense of rotation from retrograde (for depth less than $\frac{\lambda_R}{4}$) to progressive as we progress down the surface.

2.5 Analytical Expressions for Hole-Acoustic phonon interaction

In the following section, the analytic expressions for the deformation potential is introduced and the scattering rates are determined by computing the matrix element obtained using Fermi's-golden rule:

2.5.1 Deformation Potential Interaction

The deformation potential interaction arises from the local changes of the crystal potential that is caused by the displacement of the atoms due to an acoustic phonon. It follows that the divergence of the displacement, which is required to calculate the deformation potential, is given by:

$$\nabla \cdot \mathbf{u}(\mathbf{r}) = \nabla^2 \Phi = -\frac{\omega^2}{V_l} \Phi = A e^{-\alpha_{tl}y} e^{i(\beta_R z - \omega t)} \quad (2.26)$$

Since: $q = 0 \hat{t} + \beta_R \hat{k}$ (q is effectively a 1-D vector as Rayleigh waves only propagate along z -direction); $\mathbf{q} \cdot \mathbf{r} = \beta_R z$

Hence,

$$\nabla \cdot \mathbf{u}(\mathbf{r}) = A e^{-\alpha_{tl}y} e^{iq \cdot \mathbf{r}} e^{i(\omega t)} = u(y) e^{iq \cdot \mathbf{r}} (\text{dropping } e^{i(\omega t)}) \quad (2.27)$$

$$\text{Now, } U = \sqrt{\frac{\hbar}{2\rho\omega S}} (u(y)a_q + c.c)$$

Also,

$$H_{def} = -E_a \sum_q \nabla \cdot \mathbf{U} = -E_a \sqrt{\frac{\hbar}{2\rho\omega S}} \sum_q \nabla \cdot (u(y)a_q + c.c) \quad (2.28.1)$$

Hence,

$$H_{def} = -E_a \sum_q \frac{\omega^2}{V_l^2} \sqrt{\frac{\hbar}{2\rho\omega S}} u(y) (a_q e^{iq \cdot \mathbf{r}} + a_{-q}^\dagger e^{-iq \cdot \mathbf{r}}) \quad (2.28.2)$$

So that,

$$H_{def} = -C \sum_q u(y) (a_q e^{iq \cdot r} + a_{-q}^\dagger e^{-iq \cdot r}) \quad (2.28.3)$$

where, $C = E_a \frac{\omega^2}{V_l^2} \sqrt{\frac{\hbar}{2\rho\omega S}}$ and $u(y) = Ae^{-\alpha_{tl}y}$. The absorption of a phonon corresponds to the transition, $|N_q\rangle \rightarrow \langle N_q - 1|$ and emission of a phonon corresponds to the transition $|N_q\rangle \rightarrow \langle N_q + 1|$.

Now, the scattering rate expression is given as:

$$\frac{1}{\tau} = \frac{S}{(2\pi)^2} \int d^2q \frac{2\pi}{\hbar} |M^{\{e,a\}}(q)|^2 \delta(E_{k'} - E_k \pm \hbar\omega) \quad (2.29)$$

2.5.2 Matrix Element Computation

In order to evaluate the scattering rate expression we first compute matrix element $|M^{\{e,a\}}|$:

$$|M^{\{e,a\}}| = \langle k', N_q + \frac{1}{2} \pm \frac{1}{2} | H_{def} | k, N_q + \frac{1}{2} \pm \frac{1}{2} \rangle \quad (2.30.1)$$

$$|M^{\{e,a\}}| = AC \int d^3r \frac{e^{-k'l \cdot r + k \cdot r \pm q \cdot r}}{S} (y-l)^2 e^{-\alpha_{tl}y} e^{-b(y-l)} \left(N_q + \frac{1}{2} \pm \frac{1}{2} \right) \quad (2.30.2)$$

$$|M^{\{e,a\}}| = AC \int d^2r \frac{e^{-ik'l \cdot r + ik \cdot r \pm iq \cdot r}}{S} \int dy (y-l)^2 e^{-\alpha_{tl}y} e^{-b(y-l)} \left(N_q + \frac{1}{2} \pm \frac{1}{2} \right) \quad (2.30.3)$$

$$|M^{\{e,a\}}| = AC \delta_{k' - k \pm q} F \left(N_q + \frac{1}{2} \pm \frac{1}{2} \right) \quad (2.30.4)$$

[Note: F is evaluated in appendix A.II as; $= \frac{b^3}{2} \int_l^L (y-l)^2 e^{-\alpha_{tl}y} e^{-b(y-l)} dy$]

Now,

$$\sum_q |M^{\{e,a\}}|^2 = A^2 C^2 F^2 \left(n_q + \frac{1}{2} \pm \frac{1}{2} \right) \frac{1}{(2\pi)^2} \int d^2 q \delta_{\mathbf{k}' - \mathbf{k} \pm \mathbf{q}} \quad (2.30.5)$$

2.5.3 Scattering rate expression

Since, Scattering rate is given by [1]:

$$\frac{1}{\tau} = \frac{2\pi S}{\hbar} \sum_q |M^{\{e,a\}}|^2 \delta(E_{\mathbf{k}'} - E_{\mathbf{k}} \pm \hbar\omega) \quad (2.31.1)$$

Substituting the square of matrix element in above expression of scattering we get:

$$\frac{1}{\tau} = \frac{2\pi S}{\hbar} A^2 C^2 F^2 \frac{1}{(2\pi)^2} \int d^2 q \delta_{\mathbf{k}' - \mathbf{k} \pm \mathbf{q}} \delta(E_{\mathbf{k}'} - E_{\mathbf{k}} \pm \hbar\omega) \left(N_q + \frac{1}{2} \pm \frac{1}{2} \right) \quad (2.31.2)$$

So that,

$$\frac{1}{\tau} = \frac{S}{2\pi\hbar} A^2 C^2 F^2 \int d^2 q \delta_{\mathbf{k}' - \mathbf{k} \pm \mathbf{q}} \delta(E_{\mathbf{k}'} - E_{\mathbf{k}} \pm \hbar\omega) \left(N_q + \frac{1}{2} \pm \frac{1}{2} \right) \quad (2.31.3)$$

When above expression is simplified it becomes:

$$\frac{1}{\tau} = \frac{E_a^2 \omega^3 A^2}{4\pi\rho V_l^4} F^2 \int d^2 q \delta_{\mathbf{k}' - \mathbf{k} \pm \mathbf{q}} \delta(E_{\mathbf{k}'} - E_{\mathbf{k}} \pm \hbar\omega) \left(N_q + \frac{1}{2} \pm \frac{1}{2} \right) \quad (2.32)$$

In the above integral the Kronecker delta function imposes the momentum conservation condition for electron-phonon interaction, whereas the Dirac delta function imposes the energy conservation. We proceed henceforth by simplifying the integrand for absorption and emission condition separately as follows:

Case a: Condition for Absorption: The Kronecker delta in the above integrand is expressed below through the vector equation:

$$\delta_{\mathbf{k}' - \mathbf{k} - \mathbf{q}, 0} = \begin{cases} 1, & \text{if } \mathbf{k}' = \mathbf{k} + \mathbf{q} \\ 0, & \text{otherwise} \end{cases}$$

We would like to point out that, the above vectors are contained in the x-z plane (azimuthal plane). Hence the incident phonon can be absorbed from any angle ranging from 0 to 2π spanning the entire azimuthal plane

If $k' = k + q$, we can draw the vector diagram for incident angle in ranges $0 \leq \phi \leq \pi$ and $\pi \leq \phi \leq 2\pi$ respectively (we are doing this because, the argument of Dirac-delta function in eq. (2.32) is in terms of magnitude of vectors k' and k so we need to find how does the vector equation implied by Kronecker delta holds true for the condition imposed by Dirac-delta function), we draw the vector diagrams as shown in Fig 2.4:

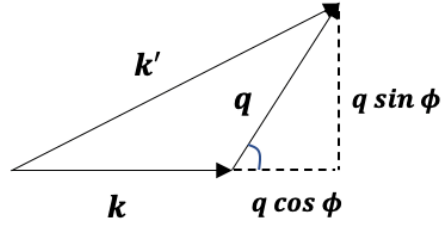


Fig. 2.4. Momentum conservation vector diagram for phonon absorption when $0 \leq \phi \leq \pi$

Applying Pythagoras theorem, we get:

$$|k'|^2 = (|k| + |q| \cos \phi)^2 + (|q| \sin \phi)^2$$

$$\text{which is equivalent to, } k'^2 = k^2 + q^2 + 2kq \cos \phi \quad (2.33)$$

Similarly, if $\pi \leq \phi \leq 2\pi$, then the vector diagram becomes as shown in Fig. 2.5:

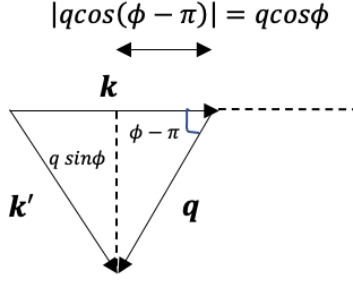


Fig. 2.5 Momentum conservation vector diagram for phonon absorption when $\pi \leq \phi \leq 2\pi$

Applying Pythagoras theorem, we get:

$$|\mathbf{k}'|^2 = (|\mathbf{k}| - |\mathbf{q}| \cos \phi)^2 + (|\mathbf{q}| \sin \phi)^2$$

which is equivalent to,

$$k'^2 = k^2 + q^2 - 2kq \cos \phi \quad (2.34)$$

Case b: Condition for Emission:

The Kronecker delta function for case of emission is given as:

$$\delta_{\mathbf{k}' - \mathbf{k} + \mathbf{q}, 0} = \begin{cases} 1, & \text{if } \mathbf{k}' = \mathbf{k} - \mathbf{q} \\ 0, & \text{otherwise} \end{cases}$$

Similar to the case of absorption, the electron can emit the phonon in any angle ranging from 0 to 2π . We consider $0 \leq \phi \leq \pi$ and $\pi \leq \phi \leq 2\pi$ separately as below:

For $0 \leq \phi \leq \pi$ the vector diagram for phonon emission is shown in Fig.2.6.

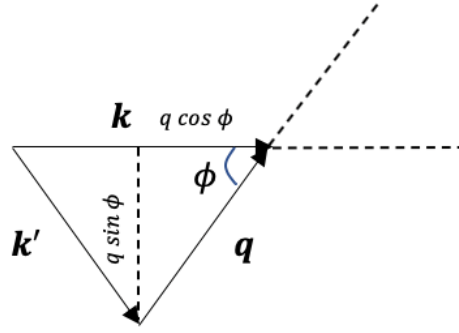


Fig. 2.6. Momentum conservation vector diagram for phonon emission when $0 \leq \phi \leq \pi$

$$|k'|^2 = (|k| - |q| \cos \phi)^2 + (|q| \sin \phi)^2$$

which is equivalent to,

$$k'^2 = k^2 + q^2 - 2kq \cos \phi \quad (2.35)$$

whereas for, $\pi \leq \phi \leq 2\pi$: the vector diagram for phonon emission is represented in Fig.7.

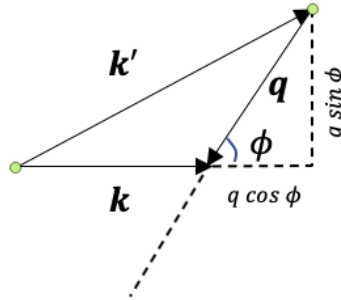


Fig. 2.7. Momentum conservation vector diagram for phonon emission when $\pi \leq \phi \leq 2\pi$

Applying Pythagoras theorem, we get:

$$|k'|^2 = (|k| + |q| \cos \phi)^2 + (|q| \sin \phi)^2$$

which is equivalent to,

$$k'^2 = k^2 + q^2 + 2kq \cos \phi \quad (2.36)$$

Now, consider the Dirac delta function for case of parabolic band:

$$\delta(E_{k'} - E_k \pm \hbar\omega_q) = \delta\left(\frac{\hbar^2 k'^2}{2m^*} - \frac{\hbar^2 k^2}{2m^*} \pm \hbar V_R q\right)$$

In the above equation we have $V_R q = \omega$. The upper “plus” sign corresponds to emission whereas the lower “minus” sign corresponds to absorption (we will adhere to this notation throughout this work)

Now the argument of above Dirac delta function can be simplified using eqs. 2.33, 2.34, 2.35 and 2.36 for emission and absorption for $0 \leq \phi \leq \pi$ and $\pi \leq \phi \leq 2\pi$ respectively as below:

For $0 \leq \phi \leq \pi$

$$\frac{\hbar^2 k'^2}{2m^*} - \frac{\hbar^2 k^2}{2m^*} = \frac{\hbar^2}{2m^*} (q^2 \mp 2kq \cos \phi) \quad (2.37)$$

and, for $\pi \leq \phi \leq 2\pi$

$$\frac{\hbar^2 k'^2}{2m^*} - \frac{\hbar^2 k^2}{2m^*} = \frac{\hbar^2}{2m^*} (q^2 \pm 2kq \cos \phi) \quad (2.38)$$

Thus, the argument of Dirac delta function can be written as:

$$= \delta\left(\frac{\hbar^2}{2m^*} (q^2 \mp 2kq \cos \phi) \pm \hbar V_R q\right) \quad (2.39.1)$$

$$= \delta\left(\frac{\hbar^2 q^2}{2m^*} \mp \frac{2\hbar^2 kq \cos \phi}{2m^*} \pm \hbar V_R q\right) \quad (2.39.2)$$

Similarly, for $\pi \leq \phi \leq 2\pi$:

$$= \delta\left(\frac{\hbar^2 q^2}{2m^*} \pm \frac{2\hbar^2 kq \cos \phi}{2m^*} \pm \hbar V_R q\right) \quad (2.40)$$

We know by the property of delta function that: $\delta(\alpha x) = \frac{1}{|\alpha|} \delta(x)$, thus applying this property above we obtain:

$$\delta(E_{k'} - E_k \pm \hbar \omega_q) = \frac{m^*}{\hbar^2 k q} \delta\left(\left(\frac{q}{2k} \pm \frac{m^* V_R}{\hbar k}\right) \mp \cos \phi\right) \quad (2.41)$$

Similarly, for $\pi \leq \phi \leq 2\pi$:

$$\delta(E_{k'} - E_k \pm \hbar \omega_q) = \frac{m^*}{\hbar^2 k q} \delta\left(\left(\frac{q}{2k} \pm \frac{m^* V_R}{\hbar k}\right) \pm \cos \phi\right) \quad (2.42)$$

Now, defining limits of integration in Eq. 2.32 as below:

$$\int d^2 q = \int_{q=q_{min}}^{q=q_{max}} \int_{\phi=0}^{\phi=2\pi} q dq d\phi = \int_{q=q_{min}}^{q=q_{max}} \int_{\phi=0}^{\phi=\pi} q dq d\phi + \int_{q=q_{min}}^{q=q_{max}} \int_{\phi=\pi}^{\phi=2\pi} q dq d\phi$$

Before proceeding further we need to determine $q = q_{min}$ and $q = q_{max}$ in the above integral for $0 \leq \phi \leq \pi$ and $\pi \leq \phi \leq 2\pi$ for emission and absorption respectively as discussed below.

Case (i): Emission ($0 \leq \phi \leq \pi$): Since, $E_{k'} - E_k = -\hbar \omega$

From Eq [3.37]: $\frac{\hbar^2 k'^2}{2m^*} - \frac{\hbar^2 k^2}{2m^*} = \frac{\hbar^2}{2m^*} (q^2 - 2kq \cos \phi) = -\hbar V_R q$

where

$$\cos \phi = \frac{q}{2k} + \frac{m^* V_R}{\hbar k} = f(q) \quad (2.43)$$

The above equation puts constraints on values that q can take for a given k (hence also on hole energy). Since, $-1 \leq \cos \phi \leq 1$, the limits of q is decided by intersection of $f(q)$ and $\cos \phi$, as shown in graph in Fig. 2.8.

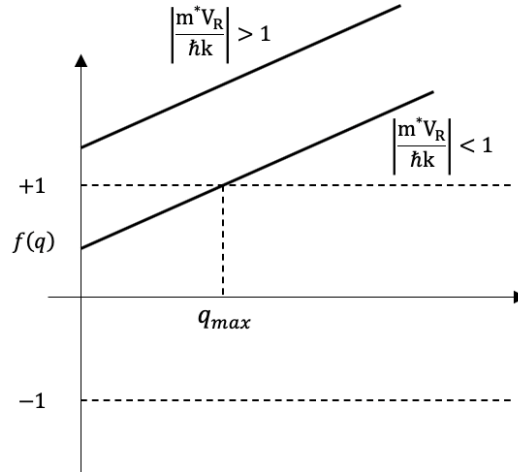


Fig. 2.8. Limitations on phonon wavevector for Case (i) of emission from $(0 \leq \phi \leq \pi)$

As we see from graph in Fig. 2.8, there are two sub-cases (a) $\left| \frac{m^*V_R}{\hbar k} \right| > 1$ and (b) $\left| \frac{m^*V_R}{\hbar k} \right| < 1$. We would like to point that case (a) and (b) translates to those holes for carrier energy less or greater than 0.3242 meV (because for $k = \frac{m^*V_R}{\hbar}$ the hole energy $\frac{\hbar^2 k^2}{2m^*} = \frac{m^*V_R^2}{2} = 0.3242$ meV).

For case (a), from fig. 3.8 we observe that Eq. (2.43) has no solution whereas for case (b) $q_{min} =$

0; q_{max} is obtained for $f(q) = +1$ and we get: $q_{max} = 2k \left(1 - \frac{m^*V_R}{\hbar k} \right)$.

Case (ii): Emission $(\pi \leq \phi \leq 2\pi)$ as shown in Fig. 2.9:

$$\cos \phi = -\frac{q}{2k} - \frac{m^*V_R}{\hbar k} = f(q) \quad (2.44)$$

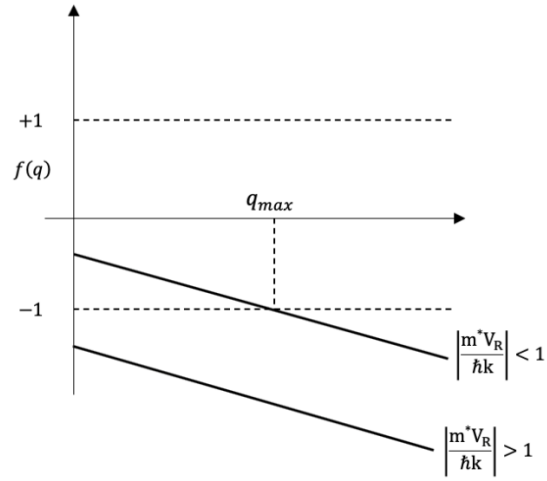


Fig. 2.9 Limitations on phonon wavevector for Case (ii) of emission from $(\pi \leq \phi \leq 2\pi)$

For case (a) (hole energy < 0.3242 meV): No solution exists because no value of q satisfies equation (44). Hence, hole with energy > 0.3242 meV cannot emit a phonon for emission angle $\pi \leq \phi \leq 2\pi$.

For case (b) (hole energy > 0.3242 meV): $q_{min} = 0$ and q_{max} is obtained for $(q) = -1$ as $q_{max} = 2k \left(1 - \frac{m^*V_R}{\hbar k} \right)$.

Case (iii): Absorption ($0 \leq \phi \leq \pi$) is plotted in Fig 3.10 from following equation as:

$$\cos \phi = -\frac{q}{2k} + \frac{m^*V_R}{\hbar k} = f(q) \quad (2.45)$$

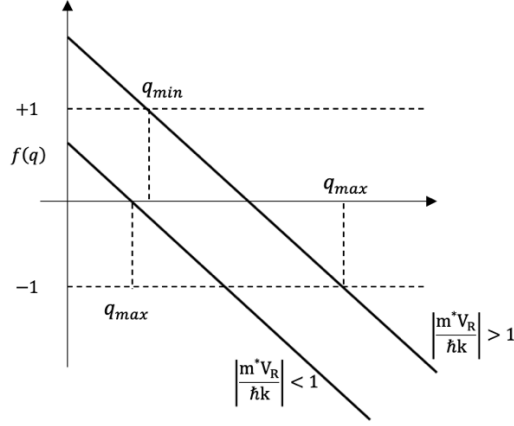


Fig. 2.10. Limitations on phonon wave vector for absorption – Case (iii) ($0 \leq \phi \leq \pi$).

For case (a) (hole energy < 0.3242 meV); q_{min} is obtained for $f(q) = +1$, we get $q_{min} = 2k \left(-1 + \frac{m^*V_R}{\hbar k} \right)$; q_{max} is obtained for $f(q) = -1$, we get $q_{max} = 2k \left(1 + \frac{m^*V_R}{\hbar k} \right)$.

For case (b) (hole energy > 0.3242 meV); $q_{min} = 0$ and q_{max} is obtained for $f(q) = -1$, we get: $q_{max} = 2k \left(1 + \frac{m^*V_R}{\hbar k} \right)$

Case (iv): Absorption ($\pi \leq \phi \leq 2\pi$): as presented in Fig. 2.11

$$\cos \phi = \frac{q}{2k} - \frac{m^*V_R}{\hbar k} = f(q) \quad (2.46)$$

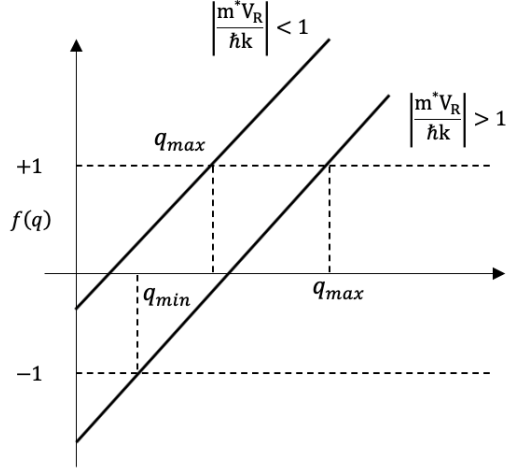


Fig. 2.11. Limitations on phonon wave vector for absorption – Case (iv) for Absorption ($\pi \leq \phi \leq 2\pi$).

For case (a) (hole energy < 0.3242 meV) q_{min} is obtained for $f(q) = -1$, we get: $q_{min} = 2k \left(-1 + \frac{m^*V_R}{\hbar k} \right)$ and q_{max} is obtained for $f(q) = +1$, we get: $q_{max} = 2k \left(1 + \frac{m^*V_R}{\hbar k} \right)$.

For case (b) (hole energy > 0.3242 meV); $q_{min} = 0$ and q_{max} is obtained for $f(q) = +1$, we get: $q_{max} = 2k \left(1 + \frac{m^*V_R}{\hbar k} \right)$.

Hence substituting $V_R q = \omega$ and applying $\delta(-x) = \delta(x)$ in Eq. 32 and setting the limits for q_{min} and q_{max} as evaluated above, we write the expressions for emission and absorption as follows:

Emission:

Case (a) (hole energy < 0.3242 meV): Emission cannot occur as has been pointed out above. Hence, we observe that the condition for emission is if the hole velocity exceeds the Rayleigh wave velocity.

Case (b) (for hole energy > 0.3242 meV)

$$\begin{aligned} \frac{1}{\tau} = & \frac{m^* E_a^2 V_R^3}{4\pi \hbar^2 k \rho V_l^4} \int_{q=0}^{q=2k\left(1-\frac{m^* V_R}{\hbar k}\right)} A_1 q^3 dq \\ & \times \left\{ \int_{\phi=0}^{\phi=\pi} d\phi \delta\left(\cos \phi - \left(\frac{q}{2k} + \frac{m^* V_R}{\hbar k}\right)\right) \right. \\ & \left. + \int_{\phi=\pi}^{\phi=2\pi} d\phi \delta\left(\cos \phi + \left(\frac{q}{2k} + \frac{m^* V_R}{\hbar k}\right)\right) \right\} \end{aligned} \quad (2.47.1)$$

$$\begin{aligned} \frac{1}{\tau} = & \frac{m^* E_a^2 V_R^3}{4\pi \hbar^2 k \rho V_l^4} \int_{q=0}^{q=2k\left(1-\frac{m^* V_R}{\hbar k}\right)} A_1 q^3 dq \\ & \times \left\{ 2 \int_{\phi=0}^{\phi=\pi/2} d\phi \delta\left(\cos \phi - \left(\frac{q}{2k} + \frac{m^* V_R}{\hbar k}\right)\right) + 2 \int_{\phi=0}^{\phi=\pi/2} d\phi \delta\left(\sin \phi - \left(\frac{q}{2k} + \frac{m^* V_R}{\hbar k}\right)\right) \right\} \end{aligned} \quad (2.47.2)$$

Absorption: Case (a) (hole energy < 0.3242 meV)

$$\begin{aligned} \frac{1}{\tau} = & \frac{m^* E_a^2 V_R^3}{4\pi \hbar^2 k \rho V_l^4} \int_{q=2k\left(-1+\frac{m^* V_R}{\hbar k}\right)}^{q=2k\left(1+\frac{m^* V_R}{\hbar k}\right)} A_1 q^3 dq \\ & \times \left\{ \int_{\phi=0}^{\phi=\pi} d\phi \delta\left(\cos \phi + \left(\frac{q}{2k} - \frac{m^* V_R}{\hbar k}\right)\right) + \int_{\phi=\pi}^{\phi=2\pi} d\phi \delta\left(\cos \phi - \left(\frac{q}{2k} - \frac{m^* V_R}{\hbar k}\right)\right) \right\} \end{aligned} \quad (2.48.1)$$

$$\frac{1}{\tau} = \frac{m^* E_a^2 V_R^3}{4\pi \hbar^2 k \rho V_l^4} \int_{q=2k\left(-1+\frac{m^* V_R}{\hbar k}\right)}^{q=2k\left(1+\frac{m^* V_R}{\hbar k}\right)} A_1 q^3 dq \quad (2.48.2)$$

$$\times \left\{ 2 \int_{\phi=0}^{\phi=\pi/2} d\phi \delta \left(\cos \phi - \left(\frac{q}{2k} - \frac{m^* V_R}{\hbar k} \right) \right) \right. \\ \left. + 2 \int_{\phi=0}^{\phi=\pi/2} d\phi \delta \left(\sin \phi - \left(\frac{q}{2k} - \frac{m^* V_R}{\hbar k} \right) \right) \right\}$$

Case (b) (hole energy > 0.3242 meV)

$$\frac{1}{\tau} = \frac{m^* E_a^2 V_R^3}{4\pi \hbar^2 k \rho V_l^4} \int_{q=0}^{q=2k \left(1 + \frac{m^* V_R}{\hbar k} \right)} A_1 q^3 dq \\ \times \left\{ \int_{\phi=0}^{\phi=\pi} d\phi \delta \left(\cos \phi + \left(\frac{q}{2k} - \frac{m^* V_R}{\hbar k} \right) \right) + \int_{\phi=\pi}^{\phi=2\pi} d\phi \delta \left(\cos \phi - \left(\frac{q}{2k} - \frac{m^* V_R}{\hbar k} \right) \right) \right\} \quad (2.49.1)$$

$$\frac{1}{\tau} = \frac{m^* E_a^2 V_R^3}{4\pi \hbar^2 k \rho V_l^4} \int_{q=0}^{q=2k \left(1 + \frac{m^* V_R}{\hbar k} \right)} A_1 q^3 dq \\ \times \left\{ 2 \int_{\phi=0}^{\phi=\pi/2} d\phi \delta \left(\cos \phi - \left(\frac{q}{2k} - \frac{m^* V_R}{\hbar k} \right) \right) + 2 \int_{\phi=0}^{\phi=\pi/2} d\phi \delta \left(\sin \phi - \left(\frac{q}{2k} - \frac{m^* V_R}{\hbar k} \right) \right) \right\} \quad (2.49.2)$$

To simplify the Dirac-delta function, we recall Eq. [8.14] from *Stroscio & Dutta* [1] as follows:

$$\int g(\phi) \delta(f(\phi) - a) d\phi = \frac{g(\phi)}{|df/d\phi|} \Big|_{\phi=\phi_0}$$

where $f(\phi_0) = a$

Evaluating the first integral,

$$\int_{\phi=0}^{\phi=\pi/2} d\phi \delta \left(\cos \phi - \left(\frac{q}{2k} \pm \frac{m^* V_R}{\hbar k} \right) \right)$$

On comparing the integral in Eq. 2.47 and 3.48 with Eq. [8.14] we observe:

$$g(\phi) = 1$$

$$f(\phi) = \cos \phi$$

$$a = f(\phi_0) = \cos \phi_0 = \left(\frac{q}{2k} \pm \frac{m^* V_R}{\hbar k} \right)$$

Hence,

$$\frac{df}{d\phi} = -\sin \phi$$

$$\left| \frac{df}{d\phi} \right|_{\phi=\phi_0} = |\sin \phi_0| = \sqrt{1 - \cos^2 \phi_0}$$

Hence,

$$\left| \frac{df}{d\phi} \right|_{\phi=\phi_0} = \sqrt{\left| 1 - \left(\frac{q}{2k} \pm \frac{m^* V_R}{\hbar k} \right)^2 \right|}$$

$$\frac{g(\phi)}{\left| df/d\phi \right|_{\phi=\phi_0}} = \frac{1}{\sqrt{\left| 1 - \left(\frac{q}{2k} \pm \frac{m^* V_R}{\hbar k} \right)^2 \right|}}$$

Similarly,

$$\int_{\phi=0}^{\phi=\pi/2} d\phi \delta \left(\sin \phi - \left(\frac{q}{2k} - \frac{m^* V_R}{\hbar k} \right) \right) = \frac{1}{\sqrt{\left| 1 - \left(\frac{q}{2k} \pm \frac{m^* V_R}{\hbar k} \right)^2 \right|}}$$

Hence substituting in the above results for Dirac-delta function and as well as for

$$A_1 = A^2 F^2 \left(N_q + \frac{1}{2} \pm \frac{1}{2} \right) = \frac{A_2}{q} \frac{b^6}{(nq+b)^6} e^{-2nql} \left(N_q + \frac{1}{2} \pm \frac{1}{2} \right) \text{ (see appendix 2.II for simplification)}$$

we obtain following expressions as plotted in Fig. 2.12:

Emission (for hole energy > 0.3242 meV):

$$\frac{1}{\tau} = \frac{m^* E_a^2 V_R^3 A_2}{\pi \hbar^2 k \rho V_l^4} \int_{q=0}^{q=2k\left(1-\frac{m^* V_R}{\hbar k}\right)} dq \frac{b^6 e^{-2\alpha_{tl}l}}{(\alpha_{tl} + b)^6} \frac{q^2}{\sqrt{\left|1 - \left(\frac{q}{2k} + \frac{m^* V_R}{\hbar k}\right)^2\right|}} (N_q + 1) \quad (2.50)$$

Absorption (for hole energy < 0.3242 meV):

$$\frac{1}{\tau} = \frac{m^* E_a^2 V_R^3 A_2}{\pi \hbar^2 k \rho V_l^4} \int_{q=2k\left(-1+\frac{m^* V_R}{\hbar k}\right)}^{q=2k\left(1+\frac{m^* V_R}{\hbar k}\right)} dq \frac{b^6 e^{-2\alpha_{tl}l}}{(\alpha_{tl} + b)^6} \frac{q^2}{\sqrt{\left|1 - \left(\frac{q}{2k} - \frac{m^* V_R}{\hbar k}\right)^2\right|}} (N_q) \quad (2.51)$$

Absorption (for hole energy > 0.3242 meV):

$$\frac{1}{\tau} = \frac{m^* E_a^2 V_R^3 A_2}{\pi \hbar^2 k \rho V_l^4} \int_{q=0}^{q=2k\left(1+\frac{m^* V_R}{\hbar k}\right)} dq \frac{b^6 e^{-2\alpha_{tl}l}}{(\alpha_{tl} + b)^6} \frac{q^2}{\sqrt{\left|1 - \left(\frac{q}{2k} - \frac{m^* V_R}{\hbar k}\right)^2\right|}} (N_q) \quad (2.52)$$

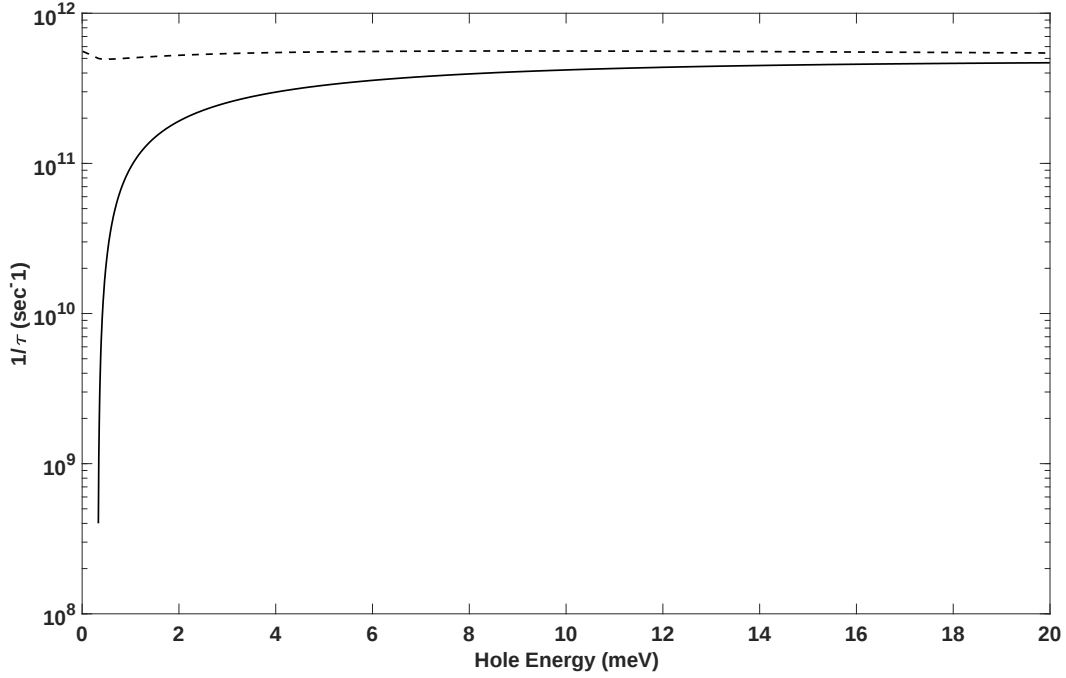


Fig. 2.12. Emission and absorption scattering rates for 2DHG at 300 K - solid line represents emission and dashed line represents absorption - for 2DHG depth of 660 pm.

These rates are nearly an order of magnitude smaller than the rates based on equipartition formula reported by Ridley et al., [35] for the case of a 3D system. Our results are based on 2DHG scattering events when the acoustic phonons are those of the surface acoustic Rayleigh waves as opposed to earlier results that assume the acoustic phonons are bulk 3D acoustic phonons. The 2D mobilities calculated based on these Rayleigh waves using the following expression for the mobility of this 2D system is calculated as:

$$\mu = \frac{e}{m} \frac{\langle E_k \tau_m \rangle}{\langle E_k \rangle} = \frac{\int_0^\infty E_k \exp(-E_k/k_B T) \tau_m dE_k}{\int_0^\infty E_k \exp(-E_k/k_B T) dE_k} = 2131.5 \text{ cm}^2/V.s$$

whereas the mean free path of hole is given by:

$$\tau_m(E_k) = \frac{1}{\left(\frac{1}{\tau_e(E_k)} + \frac{1}{\tau_a(E_k)} \right)}$$

Fig. 2.13 depicts the hole mobility due to hole—Rayleigh-wave scattering as a function of temperature with a comparison with corresponding mobility for bulk acoustic phonons as reported by Li et al. [27]. In calculating this mobility, the depth of the 2DHG ($y \approx 2/b$) has been evaluated

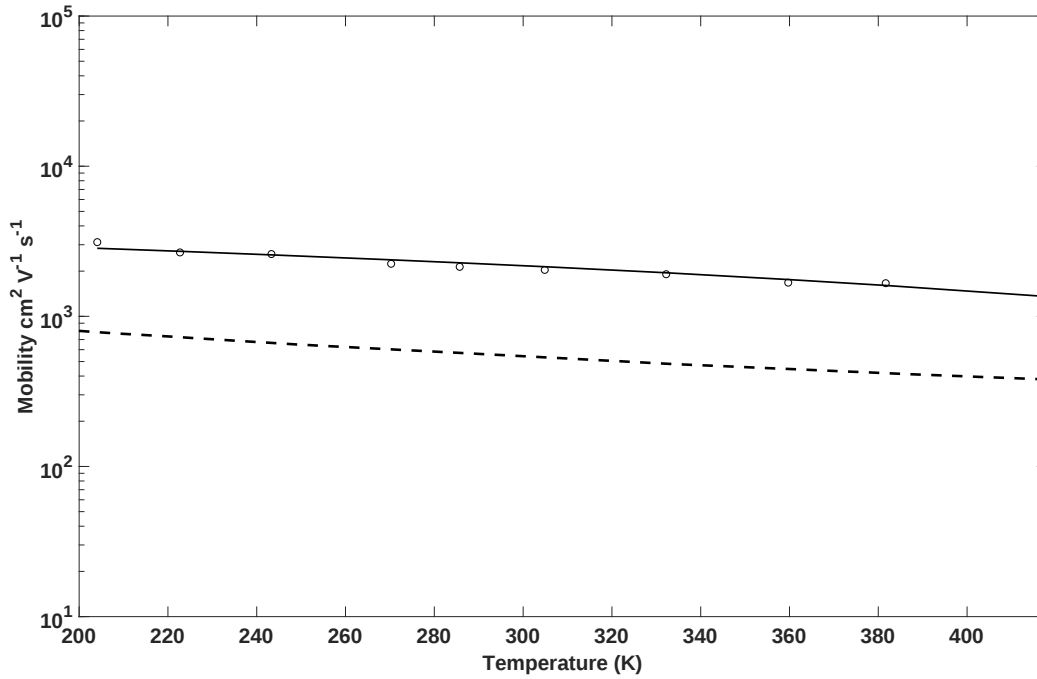


Fig. 2.13 Hole mobility due to hole—Rayleigh-wave scattering of this work (shown in solid line) compared with the mobility for hole-bulk acoustic phonon scattering (shown in dashed line) as reported in Ref. [27]. In our work the hole density dependence on temperature has been taken as reported in Ref [33] for the above temperature range.

for the corresponding hole density as reported in Ref. 33 for the above temperature range has been used in these calculations. Fig. 2.13. The mobility for the case of hole scattering from Rayleigh waves is seen to be approximately a factor of three larger than that based on hole scattering from bulk acoustic phonons. As discussed in Li et al. [27], the mobilities due to interface roughness scattering and surface impurity scattering are lower than the mobility for acoustic phonon scattering for currently realizable roughness and impurity parameters. Of course, for low level impurities and for lower levels of surface roughness, the dominant mobility-determining effect

will be due to hole-acoustic phonon scattering and, as usual, carrier-phonon scattering sets the fundamental limit on mobility.

2.6 CONCLUSIONS

Herein, we have calculated the scattering rates for holes in the 2DHG that scatter from surface acoustic waves – Rayleigh waves – as opposed to bulk 3D acoustic phonons of previous treatments for hole scattering in diamond based FETs. It is found that the scattering rates for Rayleigh wave phonons are about an order smaller than the rates based on 3D acoustic phonons. Moreover, the mobilities are found to be higher than those based on the theory for 3D acoustic phonons summarized by Ridley *et al.* [35]. These higher mobilities associated with the intrinsic acoustic phonon scattering process for Rayleigh waves as opposed to bulk acoustic phonons represent an unanticipated benefit of diamond-based devices with the 2DHG in the region where the acoustic phonons are Rayleigh waves instead of bulk acoustic phonons.

Chapter 3

PHONON-DOMINATED MOBILITIES FOR CARRIERS IN A DIAMOND FIELD EFFECT TRANSISTOR WITH A CBN OVERLAYER

© 2021 IEEE. Reprinted, with permission, from Singh, Ramji, Michael A. Strosio, and Mitra Dutta. "Phonon-Dominated Mobilities for Carriers in a Diamond Field Effect Transistor With a cBN Overlayer." *IEEE Electron Device Letters* 43, no. 1 (2021): 112-115.

3.1 Introduction

Diamond based field effect transistors (FETs) have attracted widespread attention due to the possibility of achieving high carrier mobilities of approximately $2500 \text{ cm}^2/\text{V}\cdot\text{sec}$ for the holes in the two-dimensional hole gas formed near the surface of a diamond FET [36]. Recent studies of diamond-cBN structures [37,38] have suggested the possibility of producing a two-dimensional electron gas (2DEG) in nearly lattice matched diamond-cBN heterostructures. Stimulated by the possibility of fabricating n-type FETs, we have modeled the dominant mobility-limiting carrier-phonon scattering for electrons in the 2DEG formed in the diamond near the diamond-cBN heterojunction; in determining the dominant carrier-phonon limiting mobilities, it is essential to not only model the commonly considered scattering of carriers by acoustic phonons but also carrier scattering by remote polar phonons that originate from the polar cBN overlayer; indeed, it is well established that such remote polar – also referred to as interface phonons – may play an important role in determining the electrical and optical properties of heterojunction devices [28, 39-41]. We compute the effective mobility of 2DEG limited by carrier scattering with surface acoustic

phonons and remote polar phonons. We have used the conduction band offset $\Delta E_c = 1.7 \text{ V}$ [38] at the interface.

3.2 The Two Dimensional Electron Gas

We use the 1D Schrödinger Poisson simulator [42,43] to simulate the heterostructure consisting of undoped cubic Boron Nitride (cBN) as the top overlayer over the undoped diamond substrate as shown in Fig. 1 below:

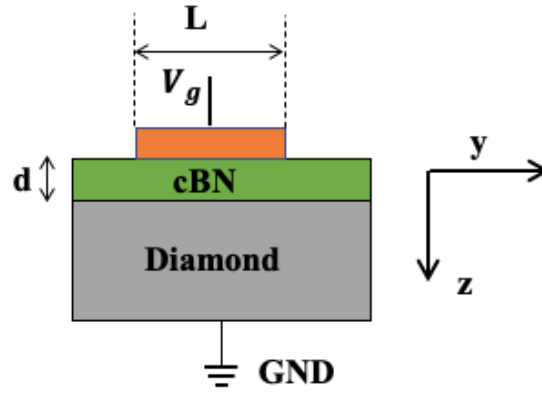


Fig. 3.1 The model cBN/Diamond FET. The cBN/Diamond interface is contained in the xy plane. The gate metal layer (orange) with an area $S = L^2$ forms a Schottky contact with the cBN layer. The diamond substrate thickness is taken to be 100 nm for calculations. © 2021 IEEE.

We find that for cBN thickness, $1.1 \leq d \leq 1.8 \text{ nm}$ the ground state energy of the electron below Fermi level. For our analysis we take $d = 1.2 \text{ nm}$. The Fig. 2 below shows the equilibrium band diagram of the cBN-diamond heterostructure.

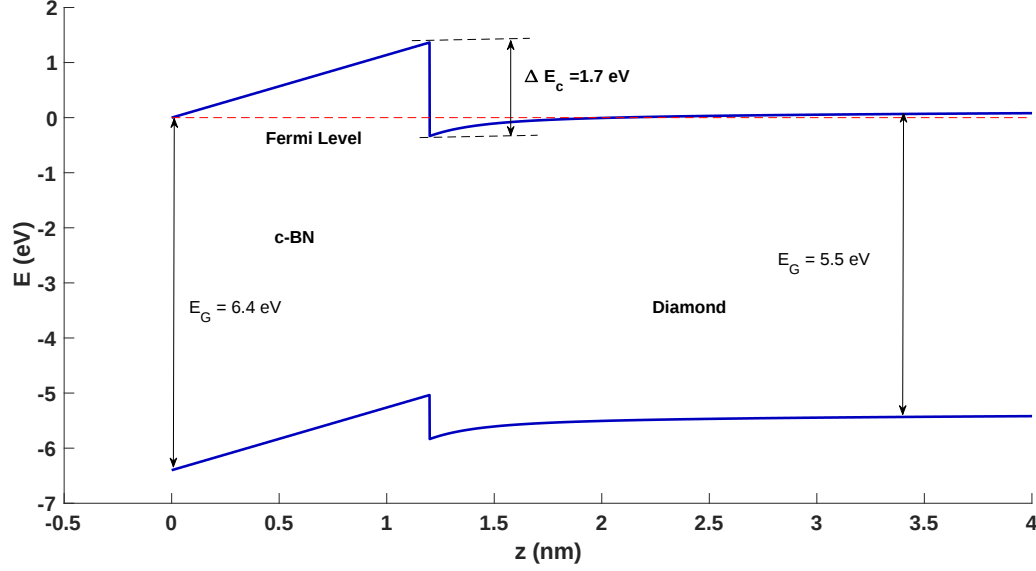


Fig. 3.2 Band diagram for cBN slab on diamond.

The electrons at the cBN/Diamond interface are confined by triangular potential well whose slope is modulated by the applied gate bias, V_g (Fig. 3(a)). Presently, there is no experimental data available on the surface density of states and Fermi level pinning for cBN. For simplicity we have assumed a 0 eV Schottky barrier (Φ_B) at the gate metal/cBN interface, we would like to point out that the inclusion of Schottky barrier height will only change the threshold voltage (the minimum applied gate voltage required to produce 2DEG).

For a total p bound states in the triangular well the volume density of electrons is given as:

$$n(z) = k_B T \frac{m^*}{\pi \hbar^2} \sum_{i=1}^p |\psi_i(z)|^2 \log \left(1 + e^{\frac{E_F - E_i}{k_B T}} \right) \quad (3.1)$$

where, m^* is the effective mass of electron, E_i is the i^{th} energy eigen value of electron, T is the absolute temperature, k_B is the Boltzmann's constant and E_F is Fermi level. The Fig. 3 shows the volume density as a function of position z .

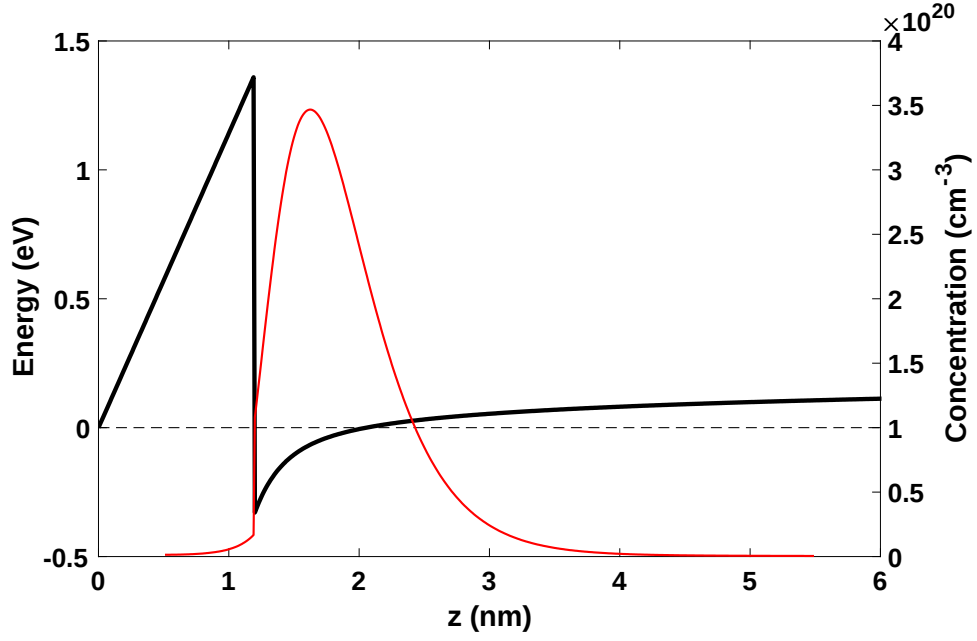


Fig. 3.3 The volume charge distribution (in red) and the conduction band profile showing the confining potential in black at 0 V gate bias and room temperature. The dashed line shows the Fermi level. (The right hand side of y-axis shows the concentration and left hand side shows the potential.) © 2021 IEEE.

For the present case we find 9 bound states out of which the ground state is 14.7 meV below the Fermi level. The first excited state is approximately $5.3 k_B T$ above the Fermi level for which the probability of occupancy less than 0.5% and hence all the states except the ground states are empty. The electrons confined by the triangular well are thus confined to the ground state but behave as plane waves in the plane which contains the cBN/Diamond interface. The electrons in the ground state subband interact with phonons to scatter from a momentum eigenstate $|\mathbf{k}\rangle$ to $|\mathbf{k}'\rangle$ where, $\mathbf{k}$ is the wavevector in the plane containing the cBN/Diamond interface. The Fig. 3.4 below shows the plot of first 3 subbands.

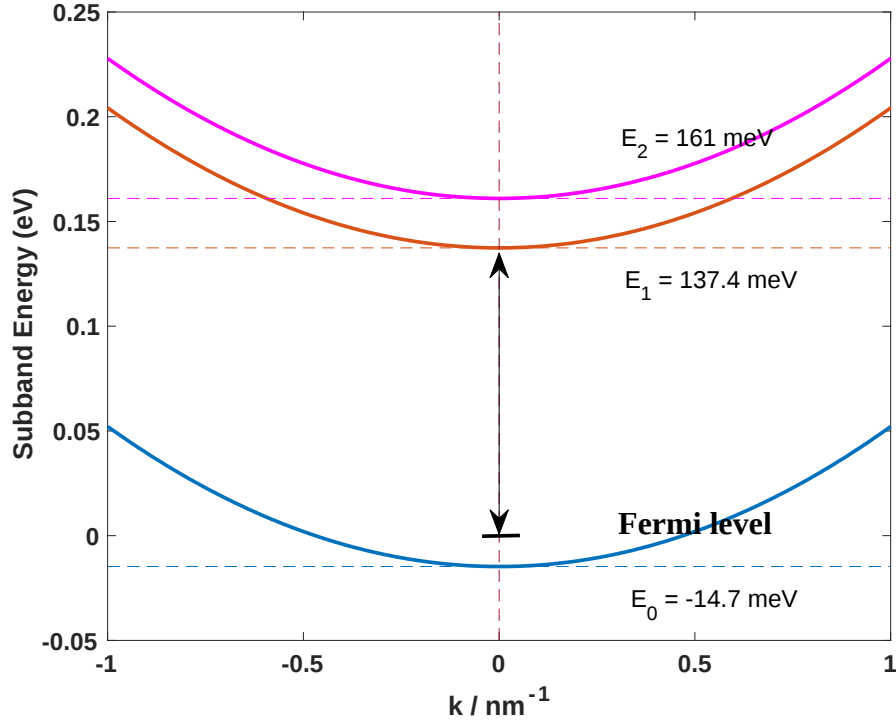


Fig. 3.4. The three lowest subbands ($E = E_n + \frac{\hbar^2 k^2}{2m^*}$) are shown depicting the 1st excited state to be approx. $5.3k_B T$ above the fermi level. The sheet density at the interface is the result of contribution from ground state electrons only at room temperature.

The 2DEG sheet density (n_s) results from the contribution of ground state electrons only. The applied gate voltage (V_g) modulates the slope of the triangular well causing the ground eigenstate to move further down below the Fermi level and the higher excited states move further upwards if the voltage is increased from 0V, accordingly the sheet density increases. The contribution of higher states to sheet density negligible.

We determine the thickness of 2DEG at a given gate bias as:

$$\Delta d = \frac{\text{Area under the volume charge density}}{\text{peak value of volume charge density } (n_{peak})} \quad (3.2)$$

3.3 Electron-Phonon interaction

3.3.1 Description of remote polar phonon

The presence of cBN/Diamond heterointerface causes localization of longitudinal optical (LO) phonons in cBN layer (medium 1) which appear as evanescent modes leaking into the underlying diamond layer (medium 2). These modes can be expressed as linear combination of symmetric and anti-symmetric components with the Fröhlich Hamiltonian as [1,5]:

$$H^{A/S} = \sum_q g(\omega, q) \frac{1}{\sqrt{2q}} e^{iq \cdot \rho} (a_q + a_{-q}^\dagger) e^{-q(z - \frac{d}{2})} \quad (3.3)$$

where,

$$g(\omega, q) = \left[\frac{4\pi\hbar e^2 S^{-1}}{\varepsilon_d^2(\partial/\partial\omega)(\varepsilon_1(\omega) f(qd/2) + \varepsilon_2(\omega))} \right]^{1/2} \quad (3.4)$$

and, $f(qd/2) \equiv \tanh\left(\frac{qd}{2}\right)$ or $\coth\left(\frac{qd}{2}\right)$ for symmetric and anti-symmetric modes, respectively.

Fig. 3.5 and 3.6 show the Fröhlich potential for symmetric and anti-symmetric case evaluated for vacuum/cBN/vacuum heterostructure. The highlighted orange curve specifically indicates the perturbing Fröhlich potential attributed to the evanescent mode leaking into the underlying diamond slab.

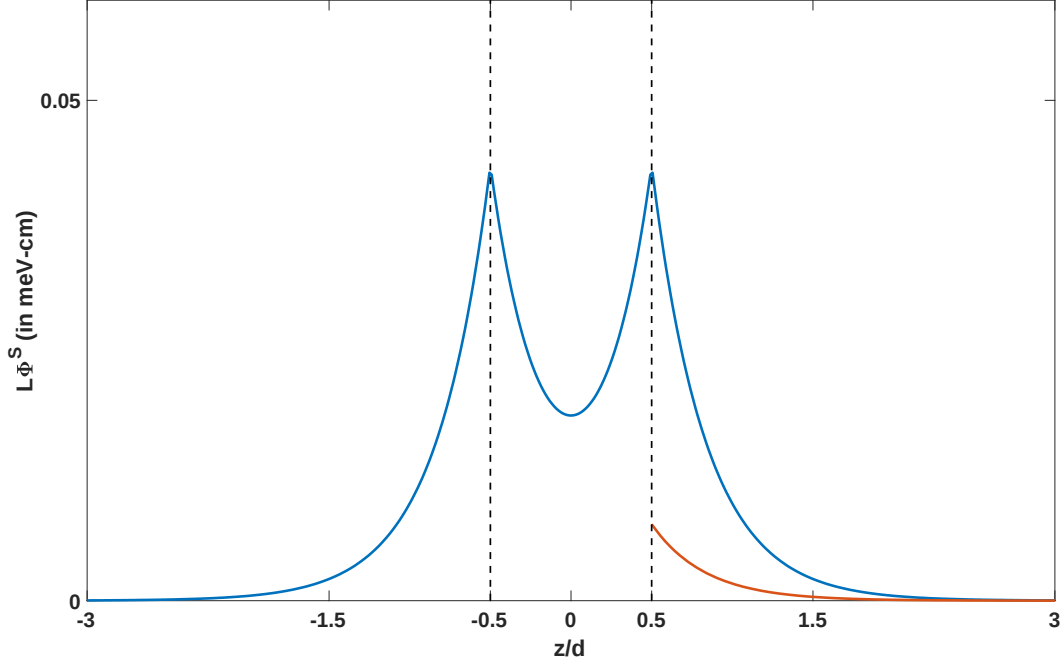


Fig. 3.5. Fröhlich potential for symmetric mode versus distance in cBN slab for $qd = 3$ is shown in blue line. The orange line shows the screened potential (for $qd = 3$) when diamond is placed in the region $z \geq d/2$, this potential is responsible for interaction with 2D electron gas at cBN-diamond interface.

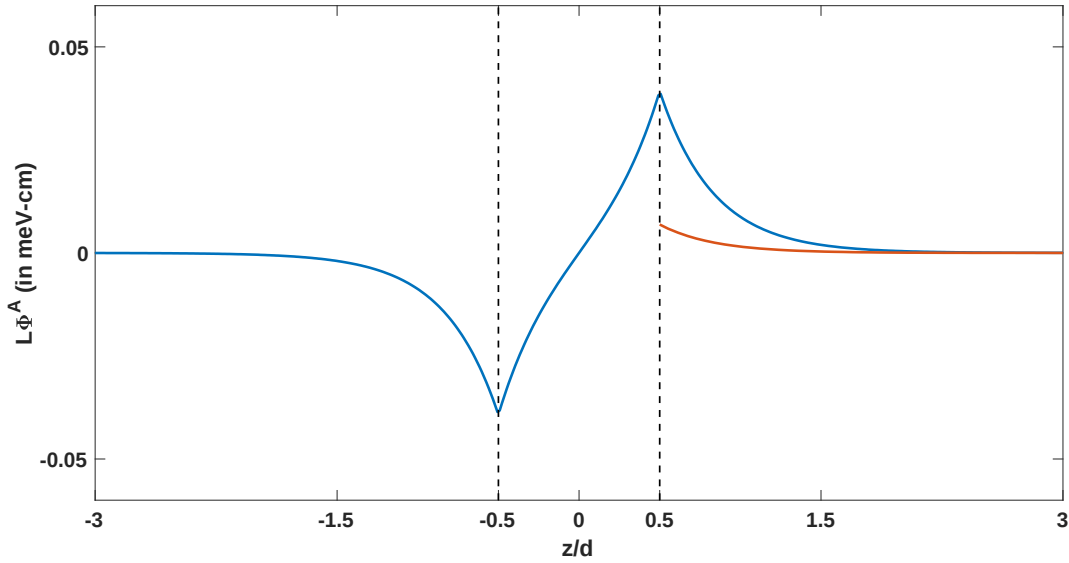


Fig. 3.6. Fröhlich potential for Anti-symmetric mode versus distance in cBN slab for $qd = 3$ is shown in blue line. The orange line shows the screened potential (for $qd = 3$) when diamond is placed in the region $z \geq d/2$, this potential is responsible for interaction with 2D electron gas at cBN-diamond interface.

In (3.4), q is the phonon wavevector, d is the cBN thickness, $S = L^2$ is the area of heterointerface, ϵ_d is the static dielectric constant of diamond ($\epsilon_d = 5.7$ [46]), ω is the phonon frequency obtained by the solution of the following secular equation for each mode:

$$\epsilon_1(\omega) f(qd/2) + \epsilon_2(\omega) = 0 \quad (3.5)$$

The frequencies obtained from the solution of above equation (9) is plotted below in Fig. 7 as a function of the phonon wave vector (q), also known as dispersion relation:

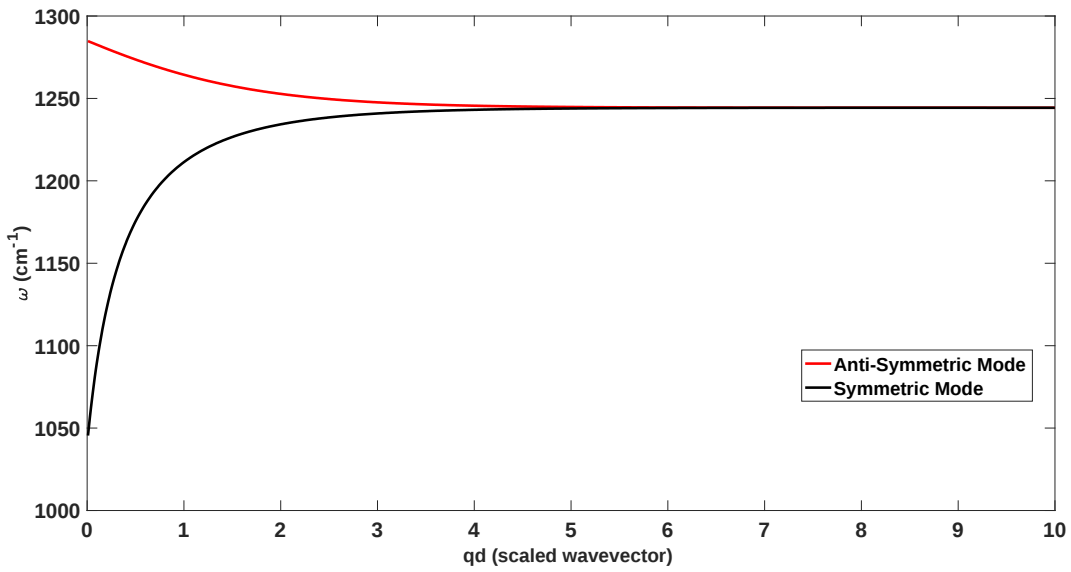


Fig. 3.7. Dispersion relation for cBN slab in vacuum for $d = 1.2$ nm.

3.3.2 Remote polar phonon scattering

To obtain the analytical expression of scattering rate of electrons in the ground state subband, we model the ground state wavefunction by Fang-Howard approximation [45,46]:

$$\psi(r) = \sqrt{\frac{b^3}{2}} (z - l) e^{-\frac{b}{2}(z-l)} \frac{e^{-ik \cdot r_{\parallel}}}{\sqrt{S}} \quad (3.6)$$

where, ‘b’ is a variational parameter, $b = \sqrt[3]{\frac{48\pi m e^2 n_s}{\epsilon_d \epsilon_0 \hbar^2}}$ [45], (n_s is numerically estimated as shown in Fig 3.8), $m = 0.57m_0$ [20] the electron effective mass for diamond, ϵ_0 is the vacuum permittivity and $\mathbf{r}_{\parallel}$ is the position vector in the x-y plane and l is the depth of 2DEG from the interface.

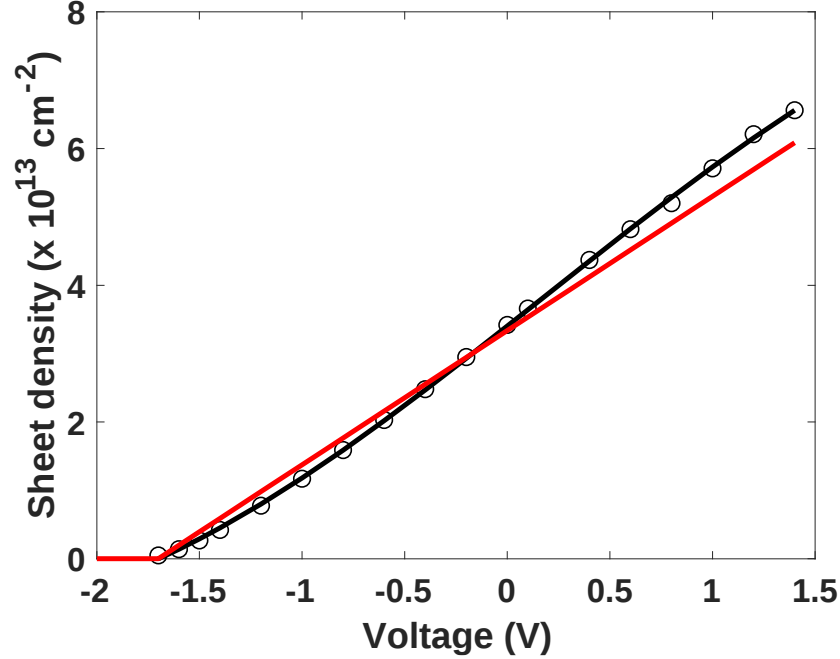


Fig. 3.8 The red curve shows the sheet charge density predicted by Gauss law $n_s = \frac{\epsilon_0 \epsilon_{c-BN}(0)}{q(d+\Delta d)} (V_g - V_{th})$ for average 2DEG thickness of 0.80 nm ($\epsilon_{c-BN}(0)=7.1$ [47]). Δd attains a maximum value of 1.2 nm at -0.4 V and decreases to 0.36 nm at 1.4 V. The black curve shows the actual sheet density obtained by integrating volume charge density in (1) w.r.t z from $z = 1.2$ nm to $z = 6$ nm. The threshold voltage $V_{th} = \Phi_B - \Delta E_c = -1.7$ V. © 2021 IEEE.

The scattering rate given by the Fermi's golden rule [1]:

$$\frac{1}{\tau_{\{e,a\}}} = \frac{S}{(2\pi)^2} \int d^2 \mathbf{q} \left(\frac{2\pi}{\hbar} \right) |M(\mathbf{q})|^2 \delta(E_{\mathbf{k}'} - E_{\mathbf{k}} \pm \hbar\omega) \quad (3.7)$$

In (3.7) the upper (plus) sign corresponds to emission and the lower (minus) sign corresponds to absorption (also the superscripts e and a corresponds to emission and absorption), we will adhere to this convention throughout the paper.

Here, $|M(q)|$ is the electron-phonon coupling matrix element given as:

$$|M(q)| = \left\langle \mathbf{k}', N_q \pm \frac{1}{2} \pm \frac{1}{2} \middle| H^{A/S} \middle| \mathbf{k}, N_q \pm \frac{1}{2} \mp \frac{1}{2} \right\rangle \quad (3.8)$$

where, $N_q = 1/(\exp(\frac{\hbar\omega}{k_B T}) - 1)$ is the phonon occupation number. Accordingly, (3.7)

becomes:

$$\frac{1}{\tau_{S,A}\{e,a\}} = \frac{b^6 S}{2\pi} \frac{m}{\hbar^3 k} \int_{q=q_1}^{q=q_2} dq \frac{g^2(\omega, q)}{q} \frac{1}{\sqrt{\left|1 - \left(\frac{q}{2k} \pm \frac{m\omega}{\hbar k q}\right)^2\right|}} \quad (3.9)$$

where, the limits of integration are determined by:

$$-1 \leq \left(\frac{q}{2k} \pm \frac{m\omega}{\hbar k q}\right) \leq 1 \quad (3.10)$$

In (3.10), ω is substituted from (3.5) to obtain the limits on q .

Now, we express the scattering rate due to emission/absorption by symmetric and anti-symmetric mode as below:

$$\frac{1}{\tau\{e,a\}} = \frac{1}{\tau_{sym}\{e,a\}} + \frac{1}{\tau_{Anti-sym}\{e,a\}} \quad (3.11)$$

and the total scattering rate is given by:

$$\frac{1}{\tau^{tot}} = \frac{1}{\tau^e} + \frac{1}{\tau^a} \quad (3.12)$$

The emission/absorption rates are plotted in Fig. 3.3(a). The mobility of electron is expressed as:

$$\mu_{op} = \frac{e \langle \tau_{Tot} \rangle}{m^*} \quad (3.13)$$

3.3.3 Scattering by surface acoustic phonon

The presence of interface modifies the bulk acoustic waves as Rayleigh waves, which are elliptically polarized waves localized near the interface with a velocity $V_R = \omega/q$ along the interface, interacts with the carrier through deformation potential resulting from distortion of the lattice causing local changes in the crystal energy bands. The particle displacement in the second quantized form is given as [46]:

$$\hat{U}(\mathbf{r}) = \sqrt{\frac{\hbar}{2\rho\omega S}} u(r)(a_{\mathbf{q}} + a_{-\mathbf{q}}^\dagger) \quad (3.14)$$

The deformation- potential interaction Hamiltonian is given as:

$$\begin{aligned} H_{def} &= E_a \sum_{\mathbf{q}} \nabla \cdot \hat{U}(\mathbf{r}) \\ &= -E_a \frac{\omega^2}{V_l^2} \sqrt{\frac{\hbar}{2\rho\omega S}} \sum_{\mathbf{q}} u(z)(a_{\mathbf{q}} e^{i\mathbf{q} \cdot \mathbf{r}_{\parallel}} + a_{-\mathbf{q}}^\dagger e^{-i\mathbf{q} \cdot \mathbf{r}_{\parallel}}) \end{aligned} \quad (3.15)$$

where, $\nabla \cdot u(r) = -\left(\frac{\omega^2}{V_l^2}\right) u(z) e^{i\mathbf{q} \cdot \mathbf{r}_{\parallel}}$; $u(z) = A e^{-\alpha_{tl} z}$; $\mathbf{r}_{\parallel}$ is the position vector in xy plane; $A^2 =$

$$\frac{A_2}{q} = \frac{2s^2 n/(n-s)^2}{q(1+s^2 n/(n-s))}, \quad n = \sqrt{1 - \frac{V_R^2}{V_l^2}} \text{ and } s = \sqrt{1 - \frac{V_R^2}{V_s^2}}, \quad E_a \text{ is the electron deformation potential}$$

(8.7eV [20]), α_{tl} is the imaginary part of the transverse wavevector of longitudinal acoustic wave, ρ is the density of diamond (3.51 gm/cm³[15]), V_l/V_s is the longitudinal/shear acoustic velocity (18.21x10⁵/12.3x10⁵ cm/sec [20]) and $V_R = 11.21 \times 10^5$ cm/sec [20].

The scattering rate is obtained from (3.7), (3.8) and (3.15) as below [46]:

$$\frac{1}{\tau^{(e,a)}} = \frac{m^* E_a^2 V_R^3 A_2}{\pi \hbar^2 k \rho V_l^4} \int_{q=q_1}^{q=q_2} dq \frac{b^6 e^{-2\alpha_{tl}l}}{(\alpha_{tl} + b)^6} \times \frac{q^2}{\sqrt{\left|1 - \left(\frac{q}{2k} \pm \frac{m^* V_R}{\hbar k}\right)^2\right|}} \left(N_q + \frac{1}{2} \pm \frac{1}{2}\right) \quad (3.16)$$

where, l is the depth of 2DEG from the interface. The limits of integration depends on threshold energy of electron [46], $E_{th} = \frac{m^* V_R^2}{2} = 0.2038$ meV. The limits for emission (upper sign) and absorption (lower sign) respectively for electron energy $E \geq E_{th}$ is:

$$q_1 = 0 \text{ and } q_2 = 2k \left(1 \mp \frac{m^* V_R}{\hbar k}\right) \quad (3.17)$$

No emission occurs for electron energy, $E \leq E_{th}$, whereas the limits for absorption for is:

$$q_1 = 2k \left(-1 + \frac{m^* V_R}{\hbar k}\right) \text{ and } q_2 = 2k \left(1 + \frac{m^* V_R}{\hbar k}\right) \quad (3.18)$$

The effective mobility due to combined effect of remote polar phonon (μ_{op}) and surface acoustic phonon (μ_{ac}) can be represented as:

$$\frac{1}{\mu_0} = \frac{1}{\mu_{ac}} + \frac{1}{\mu_{op}} \quad (3.19)$$

3.4 Discussion

The absorption rate of surface acoustic phonon is about an order of magnitude higher than the remote polar phonon at low energies which gradually decreases and become comparable for energies greater than 0.4 eV (Fig 3.9(a)).

The emission threshold for remote polar phonons is 0.154 eV, whereas, for surface acoustic phonons it is 0.2038 meV. The emission rate is on average 60 times higher for remote polar phonon than surface acoustic at 1.4V gate bias which increases to 80 times at 0 V showing higher sensitivity of acoustic phonon to electron sheet density.

From (3.9) and (3.16), it is evident that for a given energy of electron the maximum contribution to scattering is obtained from long wavelength phonons, with this approximation we can estimate that, the scattering rate expression shows a quadratic $\sim n_s^2$ variation with the 2DEG sheet density. Hence, the mobility varies as $\sim n_s^{-2}$ as is evident from Fig 9(b) (inset).

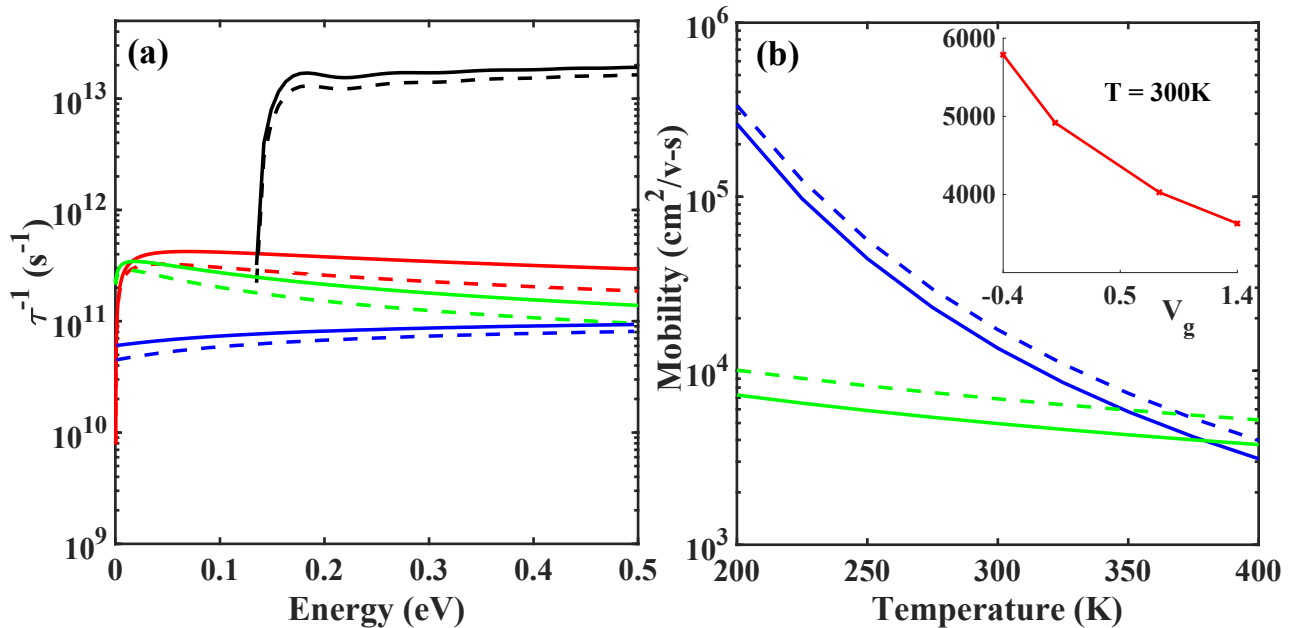


Fig. 3.9(a) Phonon scattering rate: Emission rate for remote polar phonon (black) and surface acoustic phonon (red); Absorption rate for remote polar phonon (blue) and surface acoustic phonon (green) **(b)** Mobility versus temperature for remote polar phonon (blue) and surface acoustic phonon (green) [Inset fig: effective mobility μ_0 (in $\text{cm}^2/\text{V-s}$) at various gate voltage at room temperature]. (The solid lines indicate gate voltage +1.4 V and dashed line indicates 0V). © 2021 IEEE.

3.5 Conclusion

In this paper we investigated the conditions for the formation of a 2DEG at cBN-diamond interface and found that the surface density obtained is on the order of 10^{13} cm^{-2} . At room temperature for the gate voltage increasing from 0 to +1.4V, the mean free time of electron due to remote polar phonon varies from 5.57 ps to 4.36 ps whereas for Rayleigh phonon it varies from 2.23 ps to 1.61ps, consequently the mobility limited by remote polar phonon is approximately ~2.5 times higher than Rayleigh wave (Fig. 9(b)). This result is significant because it implies that the surface acoustic phonon (Rayleigh waves) is the dominant scattering mechanism and the existence of the remote polar phonon effect does not have a major detrimental effect of the mobility. In particular, the surface acoustic phonon scattering dominates over remote polar phonon scattering for temperatures below 375 K.

Chapter 4

ACOUSTIC PHONON DECAY THROUGH THREE-PHONON PROCESSES IN 2H-SiC

[Submitted to the Journal of Electronic Materials, Springer]

4.1 Introduction

Silicon carbide (SiC) compound semiconductors have wide applications in high-performance electronic and optoelectronic devices due to their excellent electronic properties including high in-plane thermal conductivity at 300K, and high breakdown electric field [48], [49]. Modern SiC high-power and high-frequency electronics operate at densities of $3.1 - 3.22 \text{ gm/cm}^3$ [50]. Quantities such as the spontaneous and piezoelectric polarization fields allow the SiC layer to form a high-density electron channel through which electrons can flow with a saturation velocity as high as $2 \times 10^7 \text{ cm/s}$; this allows SiC-based devices to operate at high frequencies reaching RF and microwave ranges [51].

The wurtzite phase of SiC is considered both a complication and a potential feature to be utilized. Despite well-regarded efforts, many fundamental electronic and optoelectronic properties of wurtzite III–V compound semiconductors are not yet fully evaluated. The wurtzite structure of III–V semiconductors are closely related to those of the III–V zinc-blendes and can essentially coexist into crystal form during their phase transformation [52]. Similarly, as in the diamond and zinc-blende nanostructures, the wurtzite phase can be formed by considering two interpenetrating lattices. In this case, they are described as “hexagonal close packed lattices.” The nearest neighbors and next nearest neighbors are the same in the ideal wurtzite and zinc-blende structures. Figure 4.1 depicts a sample primitive unit cell of wurtzite 2H-SiC. Si atoms are represented by large blue spheres, and C atoms by smaller brown spheres.

Several studies have been proposed to improve the thermal management of semiconductor devices by realizing SiC-based substrates, as well as diamond, with high thermal conductivity. Yet, thermal conductivity is found to decrease with the rise of temperature due to optical phonon scattering caused by free carriers from dopants [53]. As the thermal properties of the materials are sensitive to the growth conditions, many in the research community have investigated growth technologies for SiC such as Hiroki et al. (2014) where they modified the I_D versus V_{DS} behavior due to self-heating effect in HEMT grown on SiC by substrate-transfer technique using hexagonal boron nitride [54].

An understanding of the electron–phonon and the phonon–phonon interaction must be incorporated to fully exploit the excellent properties of SiC materials. The propagation of acoustic phonons, particularly longitudinal acoustic phonons, is purported to be the prime mechanism for heat transport, so it is useful to understand the anharmonic decay of a given acoustic phonon mode into a final phonon mode that in general have varying velocities.

4.2 Numerical calculation of the LA phonon decay rates

Currently, thermal properties of SiC as well as their substrate interfaces are not well understood. Earlier in the semiconductor revolution, compared for silicon, the use of the 2H-SiC compound semiconductors in extensive commercial applications and high production volumes was limited; their structures were more difficult to grow than silicon and other SiC polytypes such as 4H- and 6H-SiC since their crystals have many crystal defects [55]. 2H-SiC semiconductors also tend to be more fragile which limits their growth abilities [56].

There are many theoretical studies that deal with the properties of 2H-SiC. Davydov (2004) [57] and Sarasamak et al. (2010) [58] have obtained the values of the second-order elastic constants for 2H-SiC using first principles calculations. The third-order elastic constants for 2H-SiC were calculated by Jones et al. (2014) [59] which indicates that most of the work being done to study the properties of 2H-SiC is fairly recent. No experimental data are available for the 2H-SiC polytype. We consider here the anharmonic decay of LA phonons at $T = 300\text{K}$ in an isotopically-pure SiC crystal to facilitate observing the anharmonic decay. Thus, we will neglect any scattering mechanisms and just consider the spontaneous decay process. The dispersion relations (velocity polar plots) for the modes participating in these relevant LA decay channels are depicted in Figures 4.2 and 4.3, these angular dependence of velocities are obtained as solutions of well-known Christoffel's equation. Note that these are energy and momentum conserving decay channels [60]. For the decay rates of LA modes, we will make use of the formulas from our published work provided in Ref. [60].

To examine the anisotropy of the 2H-SiC wurtzite crystal, we provide here the elastic moduli that are the elements of the compliance tensor [57]:

$$S_{ij}^{2H-SiC} = \begin{bmatrix} 0.0024 & -0.0006 & -0.0004 & 0 & 0 & 0 \\ -0.0006 & 0.0024 & -0.0004 & 0 & 0 & 0 \\ -0.0004 & -0.0004 & 0.0022 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.0070 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.0070 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.0061 \end{bmatrix}$$

We use S_{ij}^{2H-SiC} to obtain a graphical representation of the elastic properties drawn in different propagation directions as in Figure 4. It is possible from Figure 4 to classify the 2H-SiC crystal as quasi-isotropic with an anisotropy factor of 0.77 for the plane containing [001] direction. The

shape of the elastic modulus in the plane containing [100] and [010] direction is a circle (the XY plane - formed by $\vec{a}$ and $\vec{b}$ crystallographic axes), while it is slightly far from a circle in the plane containing [001] direction; thus, the elastic modulus of 2H-SiC exhibits isotropic or quasi-isotropic characteristics in the XY plane while it shows more apparent anisotropy in the plane containing [001] direction.

We consider two classes of anharmonic decay channels in the XY plane and the plane normal to the XY plane which contains the c-axis. Since the Christoffel's equation is symmetric with respect to arbitrary rotation about the z-axis, the phonon dispersion relation is identical in any arbitrary plane normal to XY plane [17], so we consider XZ plane as the plane normal to XY plane. We would like to point out that for the plane normal to XY plane, the Christoffel's equation for a plane wave solution, $\mathbf{u} = A \mathbf{e}(\mathbf{q}) \exp[i(\omega t - \mathbf{q} \cdot \mathbf{x})]$ can be written as [61]:

$$(c_{ijkl}\hat{q}_j\hat{q}_k - \rho v^2\delta_{il})e_l = 0 \quad (4.1)$$

where,

c_{ijkl} is the element of stiffness matrix, ρ is the density of the material, $\hat{q}_j$ and $\hat{q}_k$ are the direction cosines, v is the velocity of the phonon mode, $\mathbf{u}$ is the particle displacement vector, $\mathbf{e}$ is the polarization vector, A is the amplitude of particle and $\mathbf{x}$ is the position vector. The above equation is solved for all three modes shown in Fig. 4.3 one at a time to obtain the corresponding polarization vector, $\mathbf{e}$. We observe that, the in-plane polarized modes are quasi-longitudinal (shown in red) and quasi-shear (shown in blue) whereas the out-of-plane polarized mode (shown in green) is a pure shear mode. For the in-plane polarized modes we have computed the angle, α_p between the wave propagation direction unit wave vector $\hat{\mathbf{q}} = q_x\hat{i} + q_z\hat{k}$ and the polarization vector, $\mathbf{e}$ (as shown in Fig. 4.5):

$$\alpha_p(\theta) = \cos^{-1}(\hat{\mathbf{q}} \cdot \mathbf{e}) \quad (4.2)$$

where, θ is the propagation direction.

The polar plots of $\alpha_p(\theta)$ vs. θ is shown in Figs. 4.6 (a) and (b) for the in-plane quasi-longitudinal and in-plane shear mode, respectively. It is seen that for in-plane quasi-longitudinal mode:

$0^\circ \leq \alpha_p(\theta) \leq 5^\circ$ with an average value of $\approx 2.7^\circ$ and for the in-plane shear mode: $86.62^\circ \leq \alpha_p(\theta) \leq 95^\circ$ with an average value of $\approx 90.7^\circ$, so it is reasonable to assume: $\hat{\mathbf{q}} \parallel \mathbf{e}$ for the in-plane quasi-longitudinal mode and $\hat{\mathbf{q}} \perp \mathbf{e}$ for the in-plane quasi-shear mode. Thus, we treat the modes as pure modes in the plane normal to XY plane.

(1) Process 1: LA $\rightarrow$ LA + TA:

This is a spontaneous decay process in which the original LA phonon splits into a lower-energy LA phonon and a TA phonon, such that all three phonons are polarized in the same plane. We consider the XY plane and the Normal plane separately as follows.

(a) XY plane:

As shown in Fig. 4.5, consider an LA phonon with wavevector q which decays into an LA phonon with a wavevector q' and a TA phonon with a wavevector q'' . The phonon velocity is obtained by the solution of Christoffel's equation [17], as plotted in Fig. 4.2, The phonon velocities are the same in all direction in the XY plane. For an LA (TA) phonon the wavevector is parallel (normal) to the velocity, $v_l(v_t)$. We define $x = \frac{q'}{q}$, θ as the angle made by outgoing phonon q' and q and

$$r = \frac{v_l}{v_t}.$$

The momentum conservation relation: $\mathbf{q} = \mathbf{q}' + \mathbf{q}''$ yields:

$$q'' = q\sqrt{(1+x^2) - 2x \cos \theta} \quad (4.3)$$

$$\text{Whereas, the energy conservation relation gives: } \omega = \omega' + \omega'' \quad (4.4)$$

After substituting $\omega = qv_l$; $\omega' = q'v_l$ and $\omega'' = q''v_t$ in (3) and using (4), we get:

$$r(1-x) - \sqrt{(1+x^2) - 2x \cos \theta} = 0 \quad (4.5)$$

$$\cos \theta = \frac{(1+x^2) - r^2(1-x)^2}{2x} \quad (4.6)$$

Since, $-1 \leq \cos \theta \leq 1$

$$\frac{r-1}{r+1} \leq x \leq 1 \quad (4.7)$$

The angle θ as obtained in (6) is plotted vs x in Fig. 4.8 (green).

The decay rate Γ_1 which describes the anharmonic interaction of process 1 is adapted from our work in Ref. 60 as follows:

$$\begin{aligned} \Gamma_1 = \frac{\hbar \omega^5(Z)^2}{32\pi\rho^3} \int_{x_0}^1 \int_{-1}^1 dx \frac{x^3(1-x^2)^2}{v_l^7 v_t^2 ((1+x^2) - 2x \cos \theta)^{3/2}} \sin^2 \theta \cos^2 \theta \\ \times \delta(r(1-x) - \sqrt{(1+x^2) - 2x \cos \theta}) d(\cos \theta) \end{aligned} \quad (4.8)$$

$$\Gamma_1 = \frac{\hbar\omega^5}{256\pi\rho^3} \frac{(r^2 - 1)}{v_l^9} (Z)^2 \int_{x_0}^1 \frac{dx}{2x^2} (1 - x^2)^2 \times [(x + 1)^2 - r^2(1 - x)^2] [(1 + x^2) - r^2(1 - x)^2]^2 \quad (4.9)$$

where, $Z = 2\beta + 4\gamma + \lambda + 3\mu$, $\hbar$ is the reduced Planck's constant, ρ is the density and β , γ , λ , and μ are called the Lamé's constants and are given by the expressions [62]

$$\begin{aligned} \beta &= 1/35(C_{111} + 4C_{112} - 5C_{123} + 19C_{144} + 2C_{166} - 12C_{456}) \\ \gamma &= 1/35(C_{111} - 3C_{112} + 2C_{123} - 9C_{144} + 9C_{166} + 9C_{456}) \\ \lambda &= 1/5(C_{11} + 4C_{12} - 2C_{44}) \\ \mu &= 1/5(C_{11} - C_{12} + 3C_{44}) \end{aligned} \quad (4.10)$$

(b) Plane normal to XY plane:

We consider the parent phonon with wavevector q incident along the Z-axis (which is coincident with the c-axis). The phonon velocities as a function of angle with the z axis are plotted in Fig.3.

For this plane [17]:

$$r(\theta) = \frac{v_l}{v_t} \quad (4.11)$$

$$= \sqrt{\frac{c_{11}\sin^2\theta + c_{33}\cos^2\theta + c_{44} + \sqrt{[(c_{11} - c_{44})\sin^2\theta + (c_{44} - c_{33})\cos^2\theta]^2 + [(c_{13} + c_{44})\sin 2\theta]^2}}{c_{11}\sin^2\theta + c_{33}\cos^2\theta + c_{44} - \sqrt{[(c_{11} - c_{44})\sin^2\theta + (c_{44} - c_{33})\cos^2\theta]^2 + [(c_{13} + c_{44})\sin 2\theta]^2}}}$$

Substituting $r(\theta)$ in (4.5) and enforcing $-1 \leq \cos\theta \leq 1$ and $0 \leq x \leq 1$, we get a relation between θ and x (say $\theta = \theta_0(x)$), which is plotted in Fig. 4.9 (green), we use this relation to numerically solve (4.8), which simplifies as:

$$\Gamma_1 = \frac{\hbar\omega^5(Z)^2}{32\pi\rho^3} \left\{ \int_{x_0}^1 dx \frac{G_{p1}(x, \theta_0(x))}{v_l^7(\theta_0(x))v_t^2(\theta_0(x))|f'_{p1}(\theta_0(x))|} \right\} \quad (4.12)$$

where,

$$G_{p1}(x, \theta) = \frac{x^3(1 - x^2)^2}{v_l^7(\theta)v_t^2(\theta)((1 + x^2) - 2x \cos \theta)^{3/2}} \sin^2 \theta \cos^2 \theta \quad (4.13)$$

and,

$$f'_{p1}(\theta) = \frac{d}{d \cos \theta} \left(r(\theta)(1 - x) - \sqrt{(1 + x^2) - 2x \cos \theta} \right) \quad (14.14)$$

(2) Process 2: LA $\rightarrow$ TA + TA:

The parent LA phonon in process 2 decays in two TA phonons, such that (i) Polarization of all three phonons are in the same plane (Γ_2^a) or (ii) one of the TA phonon is polarized perpendicular (Γ_2^b) to the plane formed by parent LA phonon and the other daughter TA phonon.

(a) (i) Γ_2^a in XY plane:

For this case, both q' and q'' are in-plane TA phonons, such that: $\omega' = q' v_t$ and $\omega'' = q'' v_t$, where v_t is the in-plane TA phonon velocity as shown in Fig. 4.3. For this case, the energy conservation relation as in (4.4), now yield:

$$(r - x) - \sqrt{(1 + x^2) - 2x \cos \theta} = 0 \quad (4.15)$$

Thus,

$$\cos \theta = \frac{2xr + (1 - r^2)}{2x} \quad (4.16)$$

From above, we obtain:

$$\frac{r-1}{2} \leq x \leq \frac{r+1}{2} \quad (4.17)$$

(In the present case, since $\frac{r+1}{2} > 1$, so we set the upper limit to 1)

Now, the scattering rate expression is given by [60]:

$$\Gamma_a^{(2)} = \frac{\pi \hbar}{8\rho^3 V \omega} \frac{V q^3}{4\pi^2} \int_{x_1}^{x_2} \int_{-1}^1 dx \, x^2 d(\cos \theta) \left[\frac{M_{(a)}^2}{\omega' \omega''} \right] \delta(\omega - \omega' - \omega'') \quad (4.18)$$

Where,

$$M_{(a)} = \frac{qq'}{q''} \{ [\beta + \lambda + 2(\gamma + \mu)] (q' - q \cos \theta)^2 - (\beta + 2\gamma + \mu) q^2 \sin^2 \theta \} \quad (4.19)$$

Hence,

$$M_{(a)}^2 = \frac{q^6 x^2}{(1 + x^2 - 2x \cos \theta)} (C_1 (x - \cos \theta)^2 - C_2 \sin^2 \theta)^2 \quad (4.20)$$

where,

$$C_1 = [\beta + \lambda + 2(\gamma + \mu)] \text{ and } C_2 = (\beta + 2\gamma + \mu) \quad (4.21)$$

Thus,

$$\begin{aligned} \Gamma_a^{(2)} = & \frac{\hbar \omega^5}{32\pi \rho^3 (v_l^2 v_t)^3} \int_{x_1}^{x_2} \int_{-1}^1 dx \, \frac{x^3 (C_1 (x - \cos \theta)^2 - C_2 \sin^2 \theta)^2}{(1 + x^2 - 2x \cos \theta)^{3/2}} \\ & \times \delta \left((r - x) - \sqrt{(1 + x^2) - 2x \cos \theta} \right) d(\cos \theta) \end{aligned} \quad (4.22)$$

The above equation simplifies as below:

$$\Gamma_a^{(2)} = \frac{\hbar\omega^5}{32\pi\rho^3(v_l^2 v_t)^3} \int_{x_1}^{x_2} \int_{-1}^1 dx \frac{1}{16x^2(r-x)^2} \times \left\{ C_1(2x^2 - 2x\delta + (r^2 - 1))^2 + C_2(r^2 - 1)((2x - r)^2 - 1) \right\}^2 \quad (4.23)$$

(a) (ii) Γ_2^a in plane normal to XY plane (plane containing c-axis):

Using the angular variation of velocity in this plane is shown in Fig. 4.3, the numerical solution of the energy conservation relation (4.4) yields the relation between angle θ and x (say $\theta = \theta_1(x)$), which is plotted in Fig. 4.9 (in black), using this relation we simplify the scattering rate expression in (4.22) as follows:

$$\Gamma_a^{(2)} = \frac{\hbar\omega^5(Z)^2}{32\pi\rho^3} \left\{ \int_{x_0}^1 dx \frac{G_{p2}(x, \theta_1(x))}{v_l^6(\theta_1(x))v_t^3(\theta_1(x))|f'_{p2}(\theta_1(x))|} \right\} \quad (4.24)$$

where,

$$G_{p2}(x, \theta) = \frac{x^3(C_1(x - \cos \theta)^2 - C_2 \sin^2 \theta)^2}{(1 + x^2 - 2x \cos \theta)^{3/2}} \quad (4.25)$$

and,

$$f'_{p2}(\theta) = \frac{d}{d \cos \theta} \left((r(\theta) - x) - \sqrt{(1 + x^2) - 2x \cos \theta} \right) \quad (4.26)$$

(b) (i) Γ_2^b in XY plane:

It can be seen from Fig. 3, the in-plane TA phonon velocity $v_{t_1} = \frac{\omega'}{q'}$ is different from the out-of-plane velocity $v_{t_2} = \frac{\omega''}{q''}$. We have labelled in-plane TA phonon velocity as v_{t_1} , it is same as v_t used in previous paragraphs. We define the ratio of out-of-plane TA phonon velocity and in-plane TA phonon velocity as r_1 , which is given as:

$$r_1 = \frac{v_{t_2}}{v_{t_1}} \quad (4.27)$$

Hence, from the energy conservation relation (4.4), we get:

$$(r - x) - r_1 \sqrt{(1 + x^2) - 2x \cos \theta} = 0 \quad (4.28)$$

Thus,

$$\cos \theta = \frac{1}{2x} \left\{ 1 + x^2 - \frac{(r - x)^2}{r_1} \right\} \quad (4.29)$$

Now, enforcing the condition : $-1 \leq \cos \theta \leq 1$, we find the limits on x as follows:

$$x_0 \leq x \leq 1 \quad (4.30)$$

where,

$$x_0 = \frac{-(1 + r_2 r_3) + \sqrt{(1 + r_2 r_3)^2 - (1 - r_2^2)(1 - r_3^2)}}{(1 - r_3^2)} \quad (4.31)$$

$$r_2 = \frac{v_l}{v_{t_2}} \text{ and } r_3 = \frac{v_{t_1}}{v_{t_2}} \quad (4.32)$$

The general expression of scattering rate through process 2(b) channel is given by [60]:

$$\Gamma_b^{(2)} = \frac{\pi \hbar}{8\rho^3 V \omega} \frac{V q^3}{4\pi^2} \int_{x_1}^{x_2} \int_{-1}^1 dx \, x^2 d(\cos \theta) \left[\frac{M_{(b)}^2}{\omega' \omega''} \right] \delta(\omega - \omega' - \omega'') \quad (4.33)$$

where,

$$M_{(b)} = q q' [(\beta + \lambda)(q \cos \theta - q') + 2(\gamma + \mu)(q - q' \cos \theta) \cos \theta] \quad (4.34)$$

So that,

$$M_{(b)}^2 = q^6 x^2 [C_3 (\cos \theta - x) + C_4 (1 - x \cos \theta) \cos \theta]^2 \quad (4.35)$$

where,

$$C_3 = (\beta + \lambda) \text{ and } C_4 = 2(\gamma + \mu) \quad (4.36)$$

Thus,

$$\begin{aligned} \Gamma_b^{(2)} &= \frac{\hbar \omega^5}{32\pi \rho^3 v_l^6 v_{t_2}^2 v_{t_1}} \int_{x_1}^{x_2} \int_{-1}^1 dx \, \frac{x^3 [C_3 (\cos \theta - x) + C_4 (1 - x \cos \theta) \cos \theta]^2}{(1 + x^2 - 2x \cos \theta)^{1/2}} \\ &\quad \times \delta \left(\sqrt{(1 + x^2) - 2x \cos \theta} - (r_2 - r_3 x) \right) d(\cos \theta) \end{aligned} \quad (4.37)$$

which simplifies as:

$$\begin{aligned} \Gamma_b^{(2)} &= \frac{\hbar \omega^5}{32\pi \rho^3 v_l^6 v_{t_2}^2 v_{t_1}} \int_{x_1}^{x_2} dx \, x^2 \frac{|(r_2 - r_3 x)|}{(r_2 - r_3 x)} \\ &\quad \times \left[C_3 \left(\frac{(1 - x^2) - (r_2 - r_3 x)^2}{2x} \right) + C_4 \left(\frac{(1 - x^2) + (r_2 - r_3 x)^2}{2} \right) \left(\frac{(1 + x^2) - (r_2 - r_3 x)^2}{2x} \right) \right]^2 \end{aligned} \quad (4.38)$$

(b)(ii) Γ_2^b in plane normal to XY plane:

The scattering rate expression in (4.33) can also be alternately simplified as follows:

$$\Gamma_b^{(2)} = \frac{\hbar\omega^5}{32\pi\rho^3} \int_{x_1}^{x_2} \int_{-1}^1 dx \frac{x^3 [C_3(\cos\theta - x) + C_4(1 - x \cos\theta) \cos\theta]^2}{v_l^6 v_{t_1}^2 v_{t_2} (1 + x^2 - 2x \cos\theta)^{1/2}} \quad (4.39)$$

$$\times \delta(r(\theta) - x - r_1(\theta) \sqrt{(1 + x^2) - 2x \cos\theta}) d(\cos\theta)$$

In (4.39) the ratio of out-of-plane TA phonon and in-plane TA phonon velocity [61]:

$$r_1(\theta) = \frac{v_{t_2}}{v_{t_1}} \quad (4.40)$$

$$= \sqrt{\frac{2(C_{66}\sin^2\theta + C_{44}\cos^2\theta)}{c_{11}\sin^2\theta + c_{33}\cos^2\theta + c_{44} - \sqrt{[(c_{11} - c_{44})\sin^2\theta + (c_{44} - c_{33})\cos^2\theta]^2 + [(c_{13} + c_{44})^2]}}}$$

To solve (4.39), we find the numerical solution to the energy conservation relation as in (4.4)

which yields the relation between angle θ and x (say $\theta = \theta_2(x)$), which is plotted in Fig 4.9 (in red), using this relation we simplify (4.39) as:

$$\Gamma = \frac{\hbar\omega^5(Z)^2}{32\pi\rho^3} \left\{ \int_{x_0}^1 dx \frac{G_{p3}(x, \theta_2(x))}{v_l^6(\theta_2(x)) v_{t_1}^2(\theta_2(x)) v_{t_2}(\theta_2(x)) |f'_{p3}(\theta_2(x))|} \right\} \quad (4.41)$$

where,

$$G_{p3}(x, \theta) = \frac{x^3 [C_3(\cos\theta - x) + C_4(1 - x \cos\theta) \cos\theta]^2}{(1 + x^2 - 2x \cos\theta)^{1/2}} \quad (4.42)$$

and,

$$f'_{p3}(\theta) = \frac{d}{d\cos\theta} (r(\theta) - x - r_1(\theta) \sqrt{(1 + x^2) - 2x \cos\theta}) \quad (4.43)$$

The total decay rate for process 2 is: $\Gamma_2 = \Gamma_2^a + \Gamma_2^b$, we discuss the results in the following section.

Table 4.I Second- and third-order elastic constants of 2H-SiC in GPa.

C_{ij}/C_{ijk}	Jones et al. [59]
C_{11}	493
C_{12}	187
C_{44}	137
C_{111}	−2676
C_{112}	−1040
C_{123}	−1199
C_{144}	−97
C_{155}	−16
C_{456}	40.5
C_{222}	−2086
C_{122}	−1630
C_{166}	33.5

We have used the third-order elastic constants of Ref. 59 to calculate the phonon decay rates. C_{122} ,

C_{166} and C_{456} are obtained using the expressions in Ref. 63:

$$C_{122} = C_{111} + C_{112} - C_{222},$$

$$C_{166} = 1/4(3C_{222} - 2C_{111} - C_{112}) \text{ and}$$

$$C_{456} = 1/2(C_{155} - C_{144}), \text{ respectively.}$$

Table 4.II Parameters used in the present decay rates calculations.

	2H-SiC
λ ($10^{11}N/m^2$)	1.934
μ ($10^{11}N/m^2$)	1.434
β ($10^{11}N/m^2$)	−0.886
γ ($10^{11}N/m^2$)	−0.1185
ρ ($10^3kg/m^3$)	3.21

4.3 Discussion

We built this work upon the important fundamentals of electron-phonon and phonon-phonon interactions which were conveyed by Strosio and Dutta (2001) [1]. With the SiC advanced technology that allows us to build state-of-the-art systems, by exploring our decay analysis, we now have the power through quantum confinement to build and engineer low-dimensional systems that can exhibit regulated heat conduction in FETs [64] and improved performances of phonon–phonon interactions [65].

Figure 8 and Figure 9 shows the calculated decay rates in XY plane and plane normal to XY plane respectively, for process 1 (red) and process 2 (blue) by virtue of the presence of elastic anisotropy. For XY plane, it is seen that the decay rate for process 2 increases from $1.6 \times 10^3 \text{ s}^{-1}$ at 1 THz to $5.1 \times 10^6 \text{ s}^{-1}$ at 5 THz encompassing 68% of the total decay rate. The rate for process 1 varies from $0.8 \times 10^3 \text{ s}^{-1}$ at 1 THz to $2.4 \times 10^6 \text{ s}^{-1}$ at 5 THz making 32% of the total decay rate.

The branching ratios essentially remain similar throughout the frequency regions. It is observed that, process 2 is shown to dominate over process 1 by a factor of ~ 2.13 , which also reflects the difference in magnitudes of the density of states of processes 1 and 2. These aspects of our results are in agreement with previous estimations notably Klemens' [66] and our work in Ref. 60. However, for the plane normal to XY plane as shown in Fig. 9 , it is seen that the decay rate for process 1 increases from $0.8 \times 10^3 \text{ s}^{-1}$ at 1 THz to $2.4 \times 10^6 \text{ s}^{-1}$ at 5 THz encompassing 56% of the total decay rate, whereas, the rate for process 2 varies from $0.6 \times 10^3 \text{ s}^{-1}$ at 1 THz to $1.9 \times 10^6 \text{ s}^{-1}$ at 5 THz making 44% of the total decay rate. It is hence, observed that process 1 dominates over process 2 by a factor of ~ 1.28 , this is in clear contrast to XY plane. This indicates that 2H-SiC has higher thermal conductivity along the c-axis. It is seen that the decay rate for process 1 is the same in XY plane and the plane normal to the XY plane, but, process 2 decay rate in the XY plane is ~ 2.7 times higher than in the plane normal to XY plane. Fig 10 and Fig 11 show the process 2 , process 2(a) and (b) decay rates for the XY plane and normal to the XY plane, respectively. We observe that, for the XY plane the decay rate for process 2(b) dominates 2(a) by a factor of ~ 1.92 ; also, for the plane normal to XY plane the decay rate for process 2(b) dominates 2(a) by a factor of ~ 1.29 . It is the higher process 2 decay rate in XY plane than the plane normal to XY plane which increases the overall decay rate in the XY plane.

Table 4.III. Lifetimes of LA modes in 2H-SiC at 1, 3, and 5 THz.

Frequency (THz)	$\tau_T(\mu s)$ (XY plane)	$\tau_T(\mu s)$ (normal to XY plane)
1	419.88	731.58
3	1.72	3.01
5	0.134	0.23

4.4 Conclusion

The decay of longitudinal acoustic phonons into two lower-energy phonons is modeled based on the anharmonic terms in the nonlinear elasticity theory for SiC. In this paper, we have presented an estimation of spontaneous splitting of the longitudinal acoustic (LA) modes and the rates of the decay duly incorporating the variation in velocity in different propagation direction and the mechanisms by which it occurs as they are of primal importance to the development of next generation SiC devices. Evidently, the lifetime of the acoustic phonons is over an order of magnitude longer than the characteristic emission time.

Figures

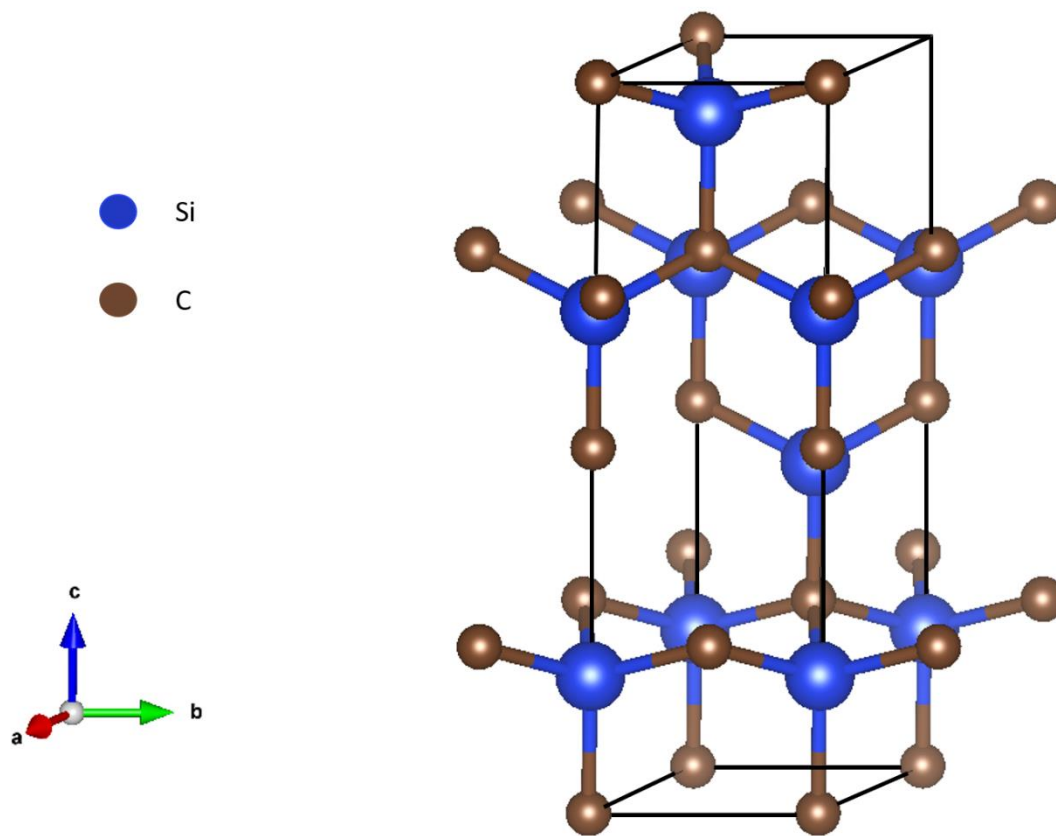


Fig. 4.1. Schematic visualization of a 2H-SiC primitive cell.

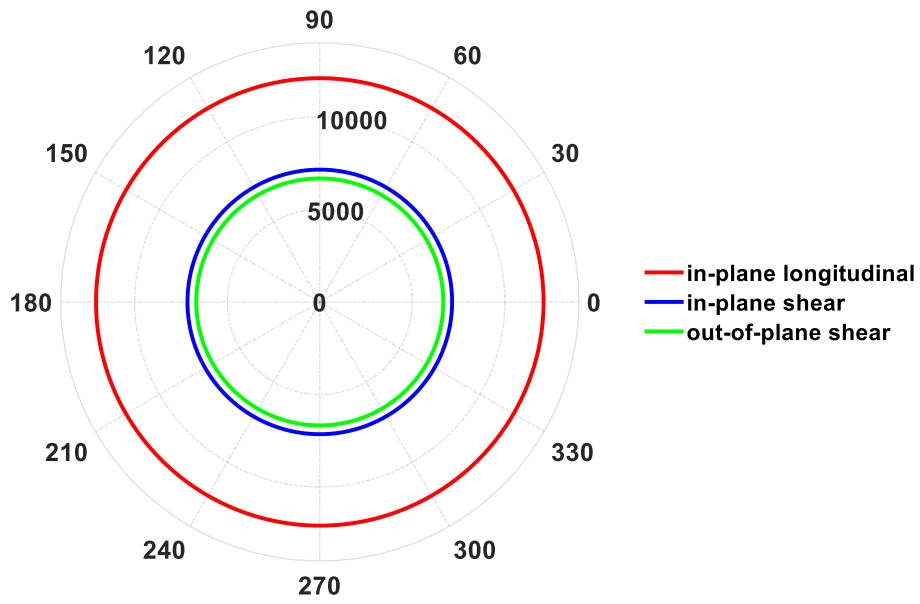


Fig. 4.2. Velocity (ms^{-1}) polar plots (dispersion relation) of bulk acoustic phonons in 2H-SiC in XY plane

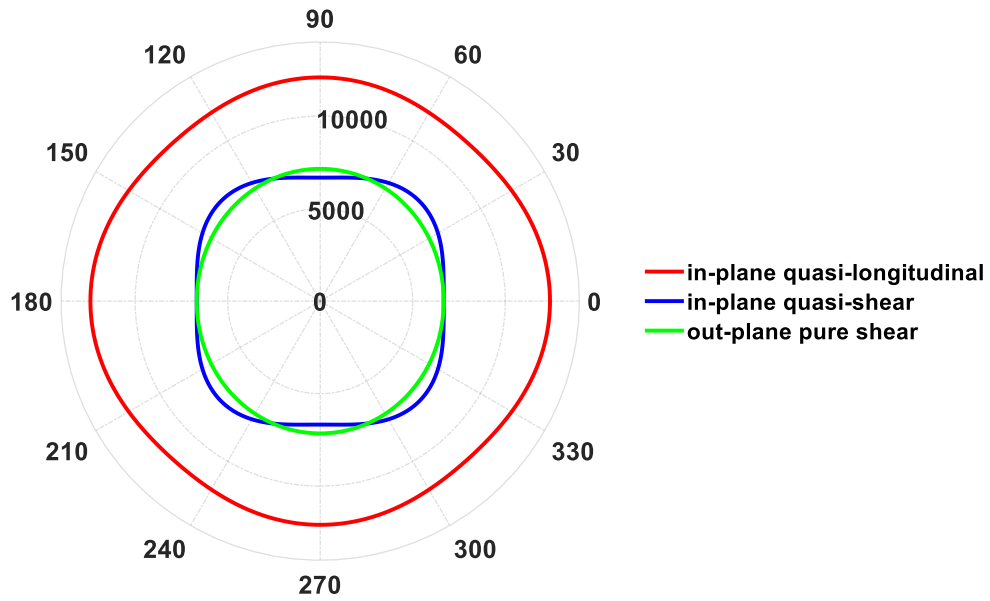


Fig. 4.3. Velocity (ms^{-1}) polar plots (dispersion relation) of bulk acoustic phonons in 2H-SiC in plane normal to XY plane (plane containing c-axis)

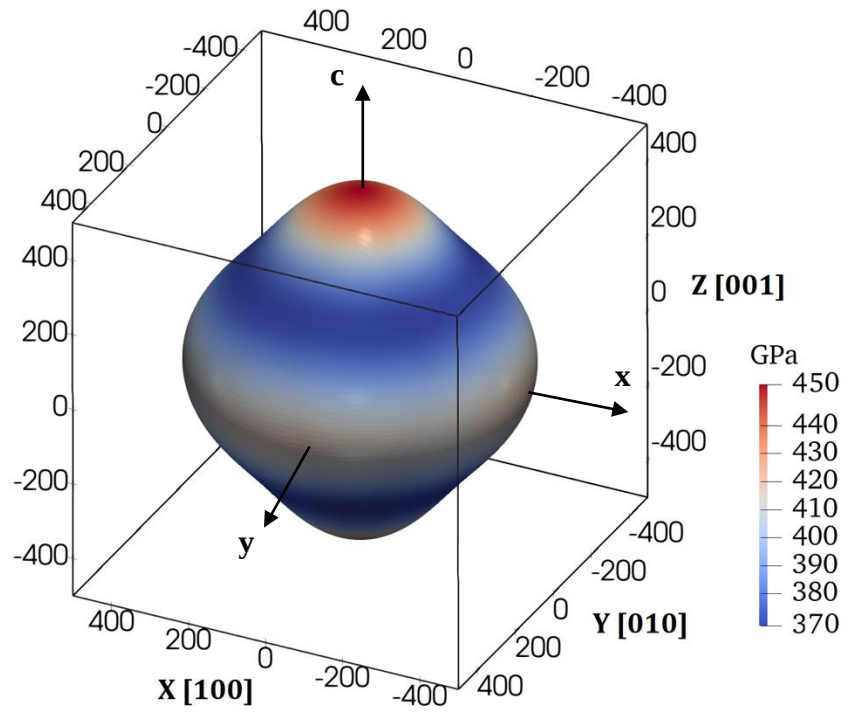


Fig. 4.4. Young's modulus of 2H-SiC wurtzite crystal in GPa. The illustration shows the predicted change in Young's modulus in the directions [100], [010], and [001].

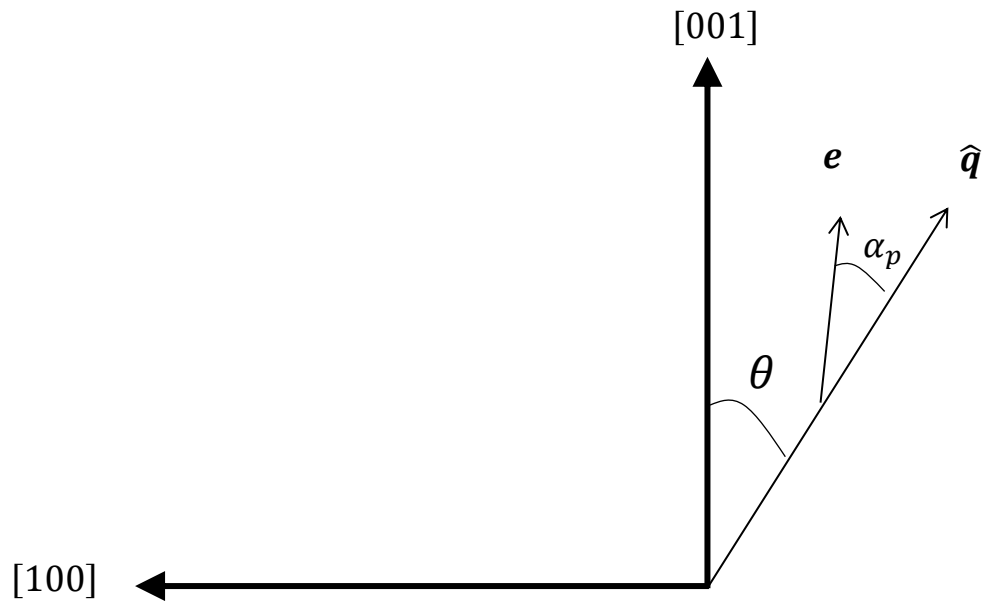


Fig. 4.5 Orientation of the polarization vector with respect to propagation direction in the plane normal to XY plane (figure not drawn to scale)

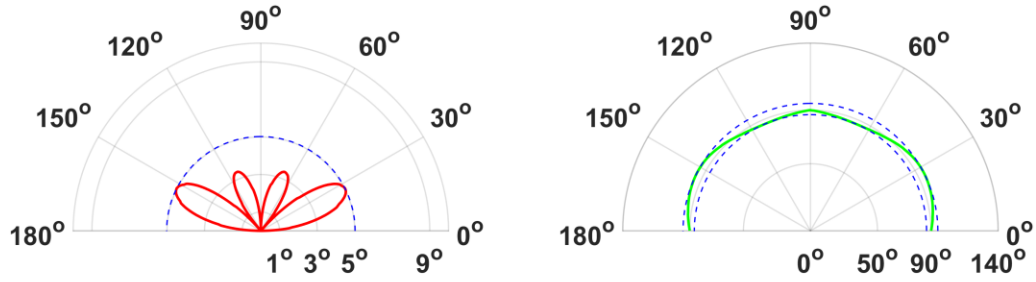


Fig. 4.6 Variation of angle α_p between the polarization vector and the propagation direction wave vector for the in-plane quasi-longitudinal and in-plane quasi-shear mode respectively in the XZ plane.

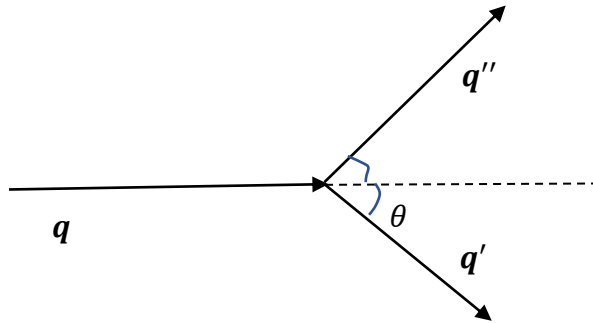


Fig. 4.7 The parent LA phonon with wavevector $\mathbf{q}$ decays into two daughter phonons with wavevector $\mathbf{q}'$ and $\mathbf{q}''$. For Process 1: $(\mathbf{q})\text{LA} \rightarrow (\mathbf{q}')\text{LA} + (\mathbf{q}'')\text{TA}$, whereas for Process 2: $(\mathbf{q})\text{LA} \rightarrow (\mathbf{q}')\text{TA} + (\mathbf{q}'')\text{TA}$.

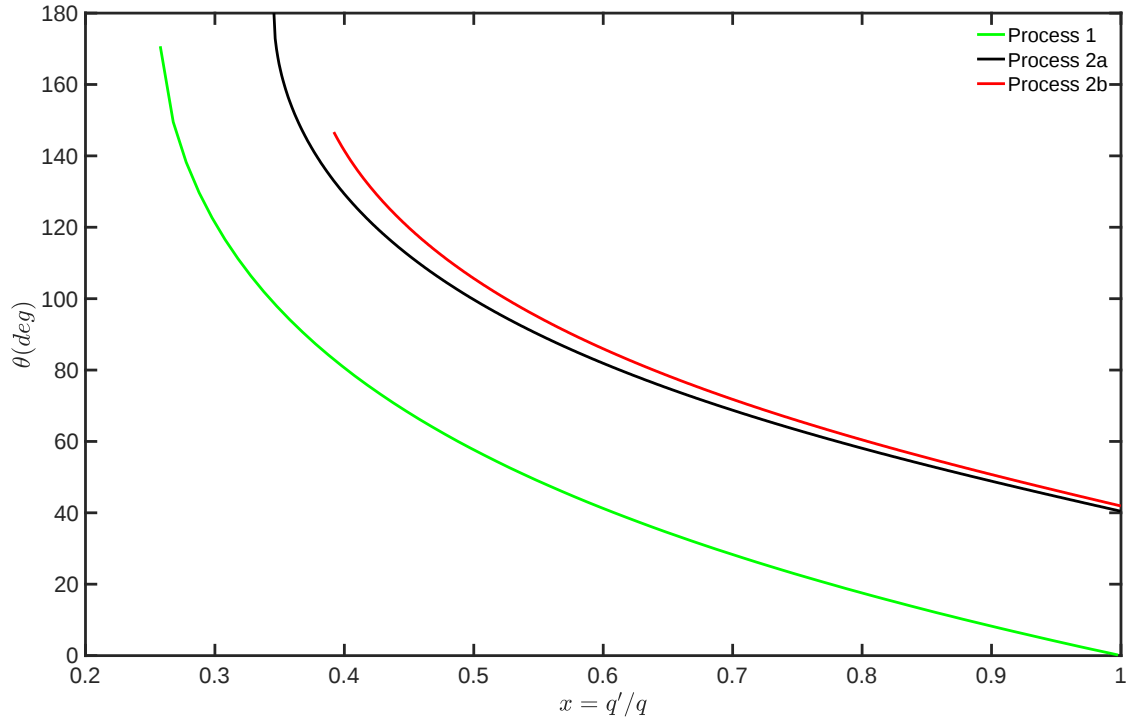


Fig. 4.8. θ (angle between q' and q) vs ratio of daughter phonon q' and parent phonon wavevector q in XY plane.

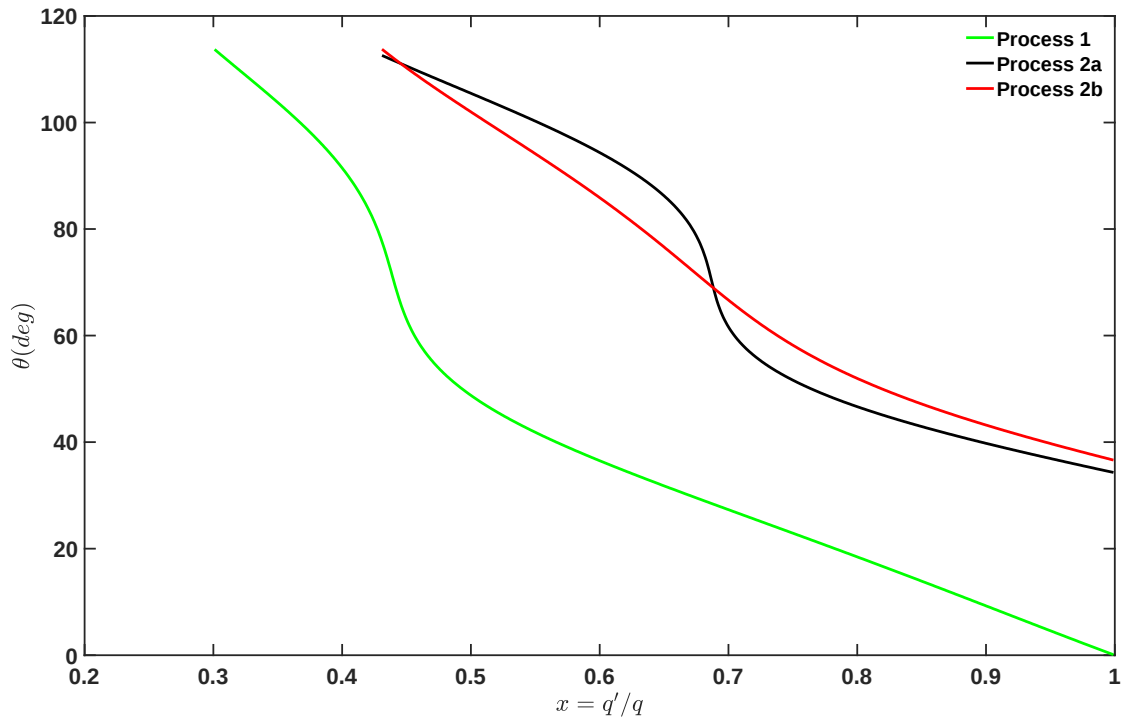


Fig. 4.9. θ (angle between q' and q) vs ratio of daughter phonon q' and parent phonon wavevector q in plane normal to XY plane

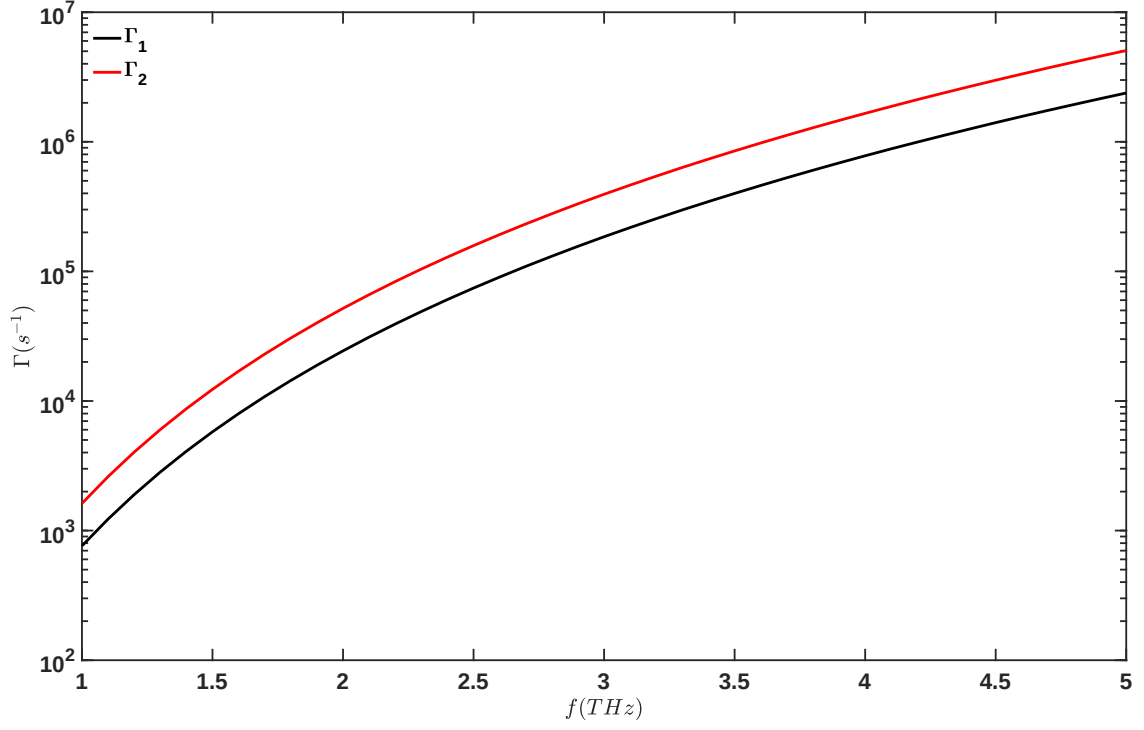


Fig 4.10. Process 1 and 2: LA phonon decay rate in XY plane for various frequencies

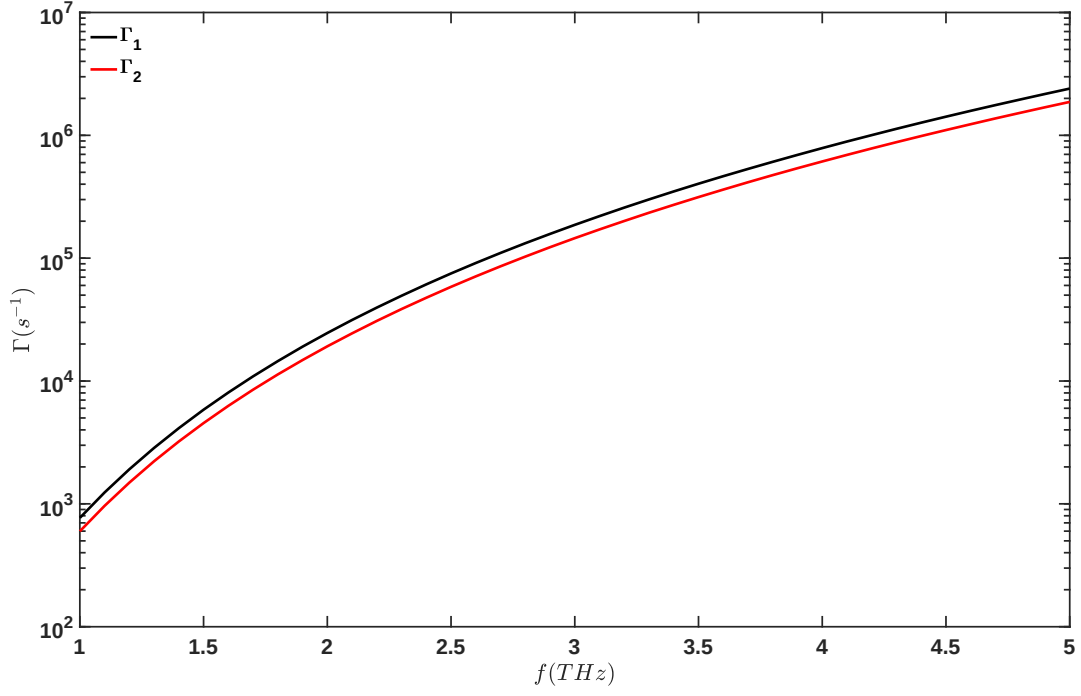


Fig 4.11. Process 1 and 2: LA phonon decay rate in plane normal to XY plane (plane containing the c-axis) for various frequencies

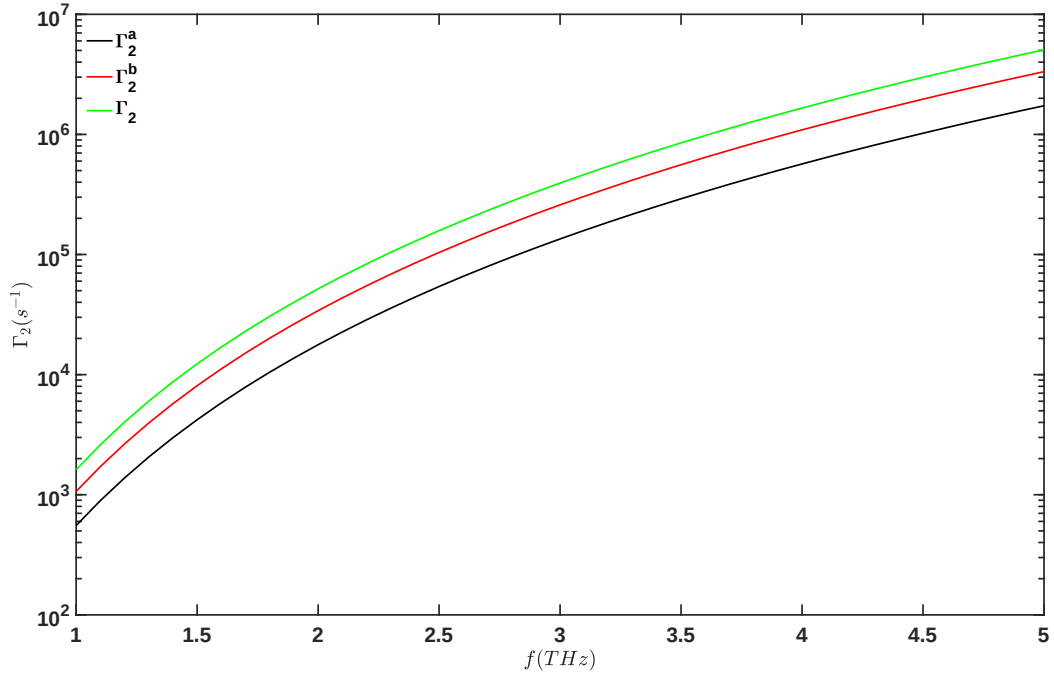


Fig 4.12. Process 2(a) and 2(b) alongwith total process 2 rate: LA phonon decay rate in XY plane for various frequencies

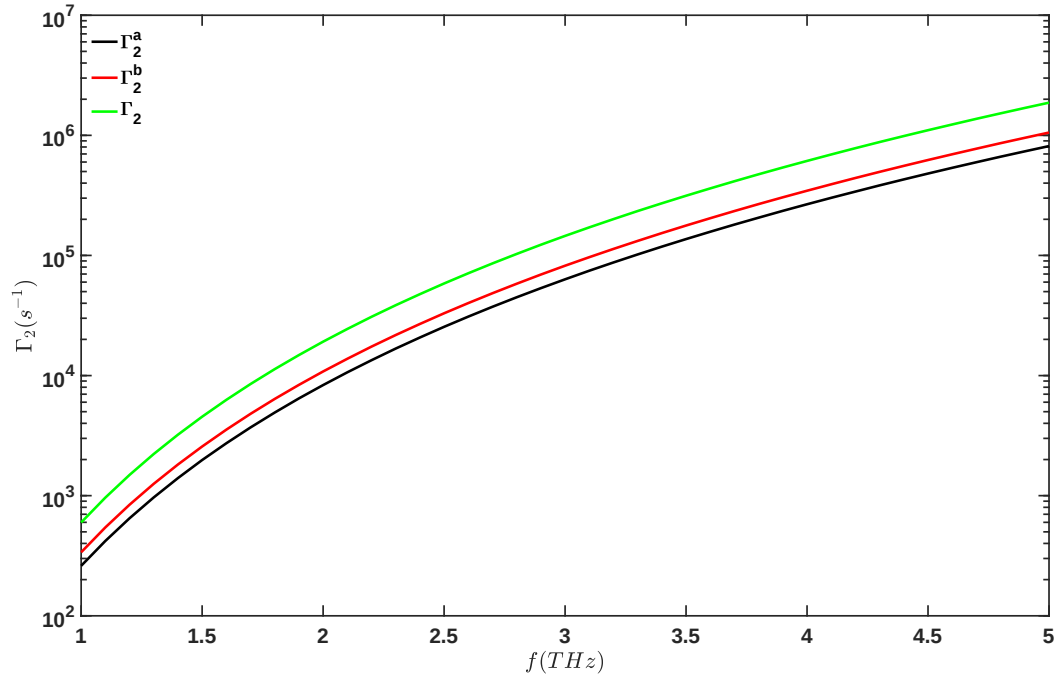


Fig 4.13. Process 2(a) and 2(b) alongwith total process 2 rate: LA phonon decay rate in plane normal to XY plane for various frequencies

Chapter 5

THORNBUR-FEYNMAN CARRIER—OPTICAL-PHONON SCATTERING RATES IN WURTZITE CRYSTALS

This is the Accepted Manuscript version of an article accepted for publication in *Journal of Physics: condensed matter*, IOP. IOP Publishing Ltd is not responsible for any errors or omissions in this version of the manuscript or any version derived from it. The Version of Record is available online at <https://doi.org/10.1088/1361-648X/abb518>.

5.1 Introduction

Recent advantages in semiconductor optoelectronics [67] and electronics [68] based upon wide bandgap materials have spurred substantial interest in the basic properties of wurtzite crystals. In addition to AlN- and GaN-based wurtzite semiconductors, BN, ZnO, CdS, CdSe, ZnS, InN, and SiC are of great interest in the electronics and optoelectronics communities. For example, the wide bandgap wurtzite crystals are attractive for high-power devices that function at elevated temperatures. Moreover, in the case of ZnO, sharp and strong excitation emission is observed even at room temperature; accordingly, ZnO portends applications in many devices, such as semiconductor lasers with wavelengths in the blue and ultraviolet as well as various electronic devices designed to work at elevated operating temperatures. As is well known, ZnO/GaN heterostructures have been studied extensively for device applications such as photodetectors and intersubband lasers using these structures have been successfully developed [68-72]. In addition, CdSe quantum dots capped with ZnS [73] and CdS quantum dots themselves may be functionalized with biomolecules and may be used as biological tags [74].

At room temperature, a principal mechanism influencing carrier interactions and transport is scattering by polar optical phonons [75]. Phonon interactions play very important roles in intersubband laser devices, especially in optical-phonon-assisted intersubband transitions [1,4,76]; thus, accurate models for carrier-phonon interactions are essential for further progress in these

fields. The macroscopic dielectric continuum model and the uniaxial model of Loudon [77] have been formulated [7,8,78,79] into models that are used widely to derive the Fröhlich interaction Hamiltonian for bulk wurtzite structures, and to perform the subsequent calculation of the associated scattering rates. A shortcoming of these previous results has been addressed in the celebrated path-integral approach in the paper of Thornber and Feynman [80] which takes into account the inadequacy of the Fermi golden rule but, unfortunately, the Thornber-Feynman (TF) model has been applied to determine corrections to the Fermi golden rule for only a few technologically important materials including AlN-based materials, GaN-based materials, and Al₂O₃ [80-81]. Herein, the TF path-integral approach is used to determine correction factors for BN, ZnO, CdS, CdSe, ZnS, InN, and SiC. It is found that these corrections to the commonly used Fermi golden rule scattering rates range in value up to an order-of-magnitude. These large corrections are due to the fact that for strong coupling constants, the mean time between carrier-phonon interactions becomes comparable with the collision time, whereas, the first-order perturbative approach underlying the Fermi golden rule assumes each instance of carrier – phonon interactions to be independent events. In the case of large Fröhlich coupling constants, the quantum interference between the phonons cannot be neglected.

5.2 Carrier—Optical-Phonon Interactions in Wurtzite Structures

In this paper, the carrier—optical phonon scattering rates for selected wurtzite semiconductors are computed using the Fermi's golden rule [1] and then compared with the path-integral-based scattering rates [80] using the Thornber-Feynman (TF) formalism.

The phonons produce macroscopic polarization fields that couple with carriers causing them to scatter as described by the Fröhlich interaction. Here, we give a brief background on the description of phonons in wurtzite crystals. Loudon (1964) proposed a model for uniaxial crystals describing phonons in wurtzite crystals. In Loudon's model, the angle between c-axis (optical axis) and the phonon wave vector $\mathbf{q}$ is denoted by θ . There are two types of phonon wave in wurtzites: (a) ordinary phonon wave – in which both electric ($\mathbf{E}$) and polarization ($\mathbf{P}$) fields are perpendicular to the c-axis and $\mathbf{q}$, respectively, for all values of θ , and (b) extraordinary waves – in which the orientation of $\mathbf{E}$ and $\mathbf{P}$ with respect to $\mathbf{q}$ and c-axis is more complicated as described below. These extraordinary phonons are of two types: (1) with A1 symmetry and associated with the perpendicular polarized vibrations with respect to c-axis and (2) E1 symmetry associated with parallel polarized vibrations with respect to c-axis. The frequency of the LO phonon wave is given by the solution to the following equation:

$$\omega_{LO}^2 = \omega_{zL}^2 \cos^2 \theta + \omega_{\perp L}^2 \sin^2 \theta \quad (5.1)$$

For a wurtzite crystal of volume V , the Fröhlich Hamiltonian (perturbation due to macroscopic polarization introduced by phonon) is given as [1, 7-8, 78-79]:

$$\begin{aligned} H_{FR}^{UA} &= i \sum_q \left\{ \frac{4\pi e^2 \hbar V^{-1}}{(\partial/\partial\omega)[\epsilon(\omega)_{\perp} \sin^2 \theta + \epsilon(\omega)_{\parallel} \cos^2 \theta]} \right\}^{1/2} \frac{1}{q} e^{iq \cdot r} (a_q + a_{-q}^{\dagger}) \\ &= \sum_q \frac{C}{q} e^{iq \cdot r} (a_q + a_q^{\dagger}) \end{aligned} \quad (5.2)$$

where,

$$C = -i \sqrt{\frac{4\pi e^2 \hbar V^{-1}}{(\partial/\partial\omega)[\epsilon(\omega)_{\perp} \sin^2\theta + \epsilon(\omega)_{\parallel} \cos^2\theta]}} \quad (5.3)$$

a_q and $a_q^{\dagger}$ represents phonon annihilation and creation operators respectively

where,

$$\epsilon(\omega)_{\perp} = \epsilon(\infty) \frac{\omega^2 - \omega_{\perp L}^2}{\omega^2 - \omega_{\perp}^2} \quad (5.4)$$

The above expression represents dielectric constant along direction perpendicular to c-axis.
and,

$$\epsilon(\omega)_{\parallel} = \epsilon(\infty) \frac{\omega^2 - \omega_{zL}^2}{\omega^2 - \omega_z^2} \quad (5.5)$$

The above expression represents the dielectric constant along the direction parallel to the c-axis.

Using these last results, it is straightforward to show that,

$$\frac{\partial \epsilon(\omega)_{\perp}}{\partial \omega} = \epsilon(\infty) (2\omega) \left[\frac{\omega_{\perp LO}^2 - \omega_{\perp TO}^2}{\omega^2 - \omega_{\perp TO}^2} \right] \quad (5.6)$$

and,

$$\frac{\partial \epsilon(\omega)_{\parallel}}{\partial \omega} = \epsilon(\infty) (2\omega) \left[\frac{\omega_{zL}^2 - \omega_z^2}{(\omega^2 - \omega_z^2)^2} \right] \quad (5.7)$$

Recalling Equation 8.24 of Ref. [1], the relation between C as in Eq (5.3) and α (Fröhlich coupling constant) is expressed as:

$$\frac{V|C|^2}{2\pi} \frac{m^*}{\hbar^3 k} = \alpha \omega \frac{1}{k} \sqrt{\frac{2m^* \omega}{\hbar}} \quad (5.8)$$

where m^* denotes the effective mass of carrier in the crystal; thus,

$$\alpha = \frac{|C|^2 V}{2\pi} \frac{1}{\omega} \frac{1}{\hbar^3} \sqrt{\frac{m^* \hbar}{2\omega}} \quad (5.9)$$

and it follows that,

$$\alpha = \frac{4\pi e^2 \hbar V^{-1}}{(\partial/\partial\omega)[\epsilon(\omega)_{\perp} \sin^2\theta + \epsilon(\omega)_{\parallel} \cos^2\theta]} \frac{1}{2\pi} \frac{V}{\omega} \frac{1}{\hbar^3} \sqrt{\frac{m^* \hbar}{2\omega}} \quad (5.10)$$

so that,

$$\alpha = \frac{2e^2}{(\partial/\partial\omega)[\epsilon(\omega)_{\perp} \sin^2\theta + \epsilon(\omega)_{\parallel} \cos^2\theta]} \sqrt{\frac{m^*}{2(\hbar\omega)^3}} \quad (5.11)$$

and

$$\alpha = \frac{2e^2}{\epsilon(\infty)(2\omega) \left[\left(\frac{\omega_{\perp,LO}^2 - \omega_{\perp,TO}^2}{(\omega^2 - \omega_{\perp,TO}^2)^2} \right) \sin^2\theta + \left(\frac{\omega_{zL}^2 - \omega_z^2}{(\omega^2 - \omega_z^2)^2} \right) \cos^2\theta \right]} \sqrt{\frac{m^*}{2(\hbar\omega)^3}} \quad (5.12)$$

This last result may be written as,

$$\alpha = \left(\frac{e^2}{\epsilon(\infty)\omega} \right) \sqrt{\frac{m^*}{2(\hbar\omega)^3}} \left[\left(\frac{\omega_{\perp,LO}^2 - \omega_{\perp,TO}^2}{(\omega^2 - \omega_{\perp,TO}^2)^2} \right) \sin^2\theta + \left(\frac{\omega_{zL}^2 - \omega_z^2}{(\omega^2 - \omega_z^2)^2} \right) \cos^2\theta \right]^{-1} \quad (5.13)$$

As is evident from the above equation, for wurtzite crystals α has an angular dependence, and for

$\theta = 0$ or $\pi/2$ the above equation reduces to isotropic case as shown below (for the isotropic case

$\omega_{zL} = \omega_{\perp L} = \omega_{LO}$; $\omega_z = \omega_{\perp} = \omega_{TO}$ and $\epsilon(0)_{\perp} = \epsilon(0)_{\parallel} = \epsilon(0)$):

$$\alpha_{cubic} = \frac{e^2}{2\hbar\omega_{LO}} \sqrt{\frac{2m^*\omega_{LO}}{\hbar}} \left[\frac{1}{\epsilon(\infty)} - \frac{1}{\epsilon(0)} \right] \quad (5.14)$$

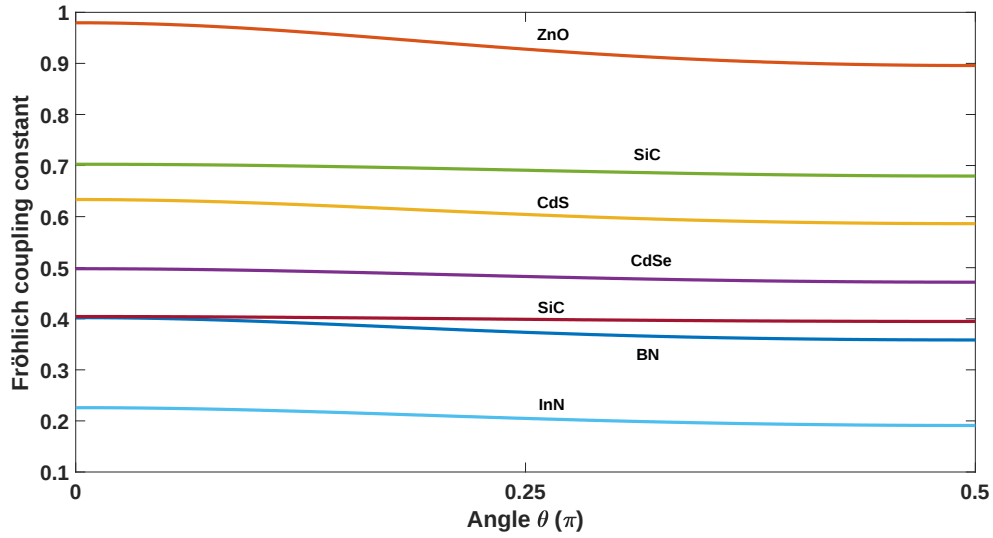


Fig. 5.1 Angular dependence of Fröhlich coupling constant on angle θ (angle between c-axis and phonon wave vector $\mathbf{q}$) for all materials under investigation.

This angular dependence is shown in Figure 5.1 which depicts the values of the Fröhlich coupling constant, α , as a function of the angle, θ , measured relative to the c-axis (which is perpendicular to the hexagonal planes) for the wurtzite crystals BN, ZnO, CdS, CdSe, ZnS, InN, and SiC, respectively. These results indicate that the anisotropy of these wurtzite crystals are only about 11% for BN, 8% for ZnO, 7% for CdS, 6% for CdSe, 3% for ZnS, 14% for InN, and 2% for SiC. As will be shown, the TF corrections to the Fermi golden rule carrier—optical-phonon scattering range from a factor of approximately 3 to 30, and it follows that the magnitude of TF correction is large compared to the anisotropy of the interaction. Accordingly, in the work the isotropic path-integral formulation of TF is compared with the Fermi golden rule interaction for phonons oriented along the c-axis. It is clear that the nearly order-of-magnitude corrections derived in this paper will be in error by only a few percent – see percentage above – due to anisotropic effects.

We provide a brief description of the Fermi golden rule model that we have used for comparison with the TF model for wurtzite crystals before proceeding further. Moving under the influence of electric field $\mathbf{E}$, the electron accelerates as it gains energy from the electric field until the energy of an electron (E_k) becomes comparable to the energy of optical phonon ($\hbar\omega_{LO}$), after which the electron loses energy by emitting optical phonons every τ^e seconds moving with a steady state velocity v . The energy gained from the electric field is balanced by the energy loss to lattice by the emission of phonons; hence, $\hbar\omega_{LO} = eE$ in steady state. The mean time between “collisions” is thus, $v\tau^e$. We must point out that, this model assumes any consecutive carrier – phonon interactions (or collisions) to be independent event separated in time and space and does not take into account the interference between the emitted phonons.

The expression for scattering rate ($1/\tau^e$) for wurtzite crystals is given as in [79]:

$$\frac{1}{\tau^e} = \frac{1}{\pi a_B} \sqrt{\frac{m^* \hbar}{2m_0}} \int_0^\pi \frac{(N_q + 1) \sin\theta}{\sqrt{\omega} \left[\frac{\partial \epsilon_\perp}{\partial \omega} \sin^2\theta + \frac{\partial \epsilon_z}{\partial \omega} \cos^2\theta \right]} \int_0^{2\pi} \frac{\sigma}{\sqrt{\frac{E_k}{\hbar\omega} \cos^2 \widehat{\mathbf{kq}} - 1}} d\phi d\theta \quad (5.15)$$

where, $N_q = \frac{1}{e^{\hbar\omega/k_B T} - 1}$ represents the phonon occupation number, a_B is the Bohr radius, ϕ is the azimuthal angle and $\cos \widehat{\mathbf{kq}} = \sin\theta \sin\theta_k \sin\phi + \cos\theta \cos\theta_k$, where θ_k is the initial electron incident angle with c-axis. We would like to point out that there is a negligible dependence of $\frac{1}{\tau^e}$ on θ_k [79], hence, we have used $\theta_k = 0$ in the current paper. Also,

$$\sigma = \begin{cases} 0 & \text{for } \cos \widehat{\mathbf{kq}} < \sqrt{\hbar\omega/E_k} \\ 2 & \text{otherwise} \end{cases}$$

From discussion above, the energy lost by electron per unit distance can be given as:

$$\frac{\hbar\omega_{LO}}{v\tau^e} \quad (5.16)$$

Here, we have determined ω_{LO} as below:

$$\omega_{LO}^2 = \omega_{zL}^2 \cos^2 \theta_{avg} + \omega_{\perp L}^2 \sin^2 \theta_{avg} \quad (5.17)$$

where, θ_{avg} is the angle corresponding to the average value of Fröhlich coupling constant $\left(\frac{2}{\pi} \int_0^{\pi/2} \alpha(\theta) d\theta\right)$ derived from Fig.5.1. These values have been tabulated in Table. 5.I for all materials under investigation.

Finally, for an electron initially in the state $|\phi_m\rangle$ makes a transition to $|\phi_n\rangle$, due to perturbation H_{el-ph} introduced by carrier – phonon interaction the Fermi golden rule predicts the transition probability per unit time as (Stroscio and Dutta [Ref 1]):

$$= \left(\frac{2\pi}{\hbar}\right) |\langle\phi_m|H_{el-ph}|\phi_n\rangle|^2 \delta(E_m - E_n \pm \hbar\omega_{LO}) \quad (5.18)$$

The above equation leads to Eq. (15) when $H_{el-ph} = H_{Fr}^{UA}$ and $|\phi_m\rangle \equiv |\mathbf{k}, N_q\rangle$ and $|\phi_n\rangle \equiv |\mathbf{k}', N_q - 1\rangle$ (where, $\mathbf{k}$ and $\mathbf{k}'$ is the initial and final electron wave vector). As discussed in Ref. 1, Eq. 5.18 is valid only for time scale, $t \gg \frac{2\hbar}{E_m - E_n} \left(= \frac{2}{\omega_{mn}}\right)$; for the present case, the phonon energy lies in the range from 0.03 – 0.15 eV for the materials under investigation as is evident from Table I. Hence, the mean free time would be of the order of 10^{-15} sec [Ref 80]; thus, in the present case quantum interference between emitted phonon can neither be neglected nor the phonon emission can be regarded as independent events.

In order to obtain non-perturbative scattering rate corrections to the Fermi golden rule scattering rates, the path-integral formulation of TF [80] is used to determine the non-perturbative scattering rates for that for BN, ZnO, CdS, CdSe, ZnS, InN, and SiC. As we have discussed above, these corrections to the commonly used Fermi golden rule scattering rates range in value up to an order-of-magnitude. In materials with high Fröhlich coupling constant, the collision time becomes comparable to the mean time between collision and it is inadequate to apply the Fermi golden rule which treats phonon collisions as independent events.

Thornber and Feynman [80] address the specific problem of determining the expectation value of the velocity of a carrier interacting with an electric field inside a semiconductor. In this case, the charge carrier gains kinetic energy from the applied electric field and the electron loses energy to the lattice by interacting with polar optical phonons. Using Fröhlich's polaron model and the Feynman path-integral method, the expression for the electric field, $\mathbf{E}$, needed to balance the net loss of energy per unit distance to the polar crystal to maintain the steady-state velocity $\mathbf{v}$ of carrier is given by [80]:

$$E = \frac{4\alpha}{v^2 \beta \pi^{1/2} \sinh\left(\frac{1}{2}\beta\right)} \int_0^{v(\sqrt{\beta})v_0/w_0} x^2 dx \int_0^\infty ds \frac{\cos\left(\frac{1}{2}\beta s\right)}{[A(s)]^{3/2}} \exp\left(-x^2 \frac{s^2 - 1}{2A(s)}\right) \times \left[\cos\left(\frac{x^2 s}{A(s)}\right) - s \sin\left(\frac{x^2 s}{A(s)}\right) \right] \quad (5.19)$$

where:

$$A(s) = s^2 + 1 + \frac{4}{\beta} \frac{v_0^2 - w_0^2}{w_0^2 v_0} \frac{\cosh\left(\frac{1}{2}\beta v_0\right) - \cos\left(\frac{1}{2}sv_0\beta\right)}{\sinh\left(\frac{1}{2}\beta v_0\right)}$$

In above expression, α is the Fröhlich coupling constant, $\beta = \frac{\hbar\omega_{LO}}{kT}$ (ratio of optical phonon energy to thermal energy), x and s are dummy variables representing carrier coordinate variables as used in evaluating the path integral, v_0 and w_0 are variational parameters defined in [81] which are obtained after minimizing the ground state energy of polaron.

The $E(v)$ function of the above equation represents a monotonically increasing function starting from $E = 0$ at $v = 0$ and increasing to $E = E_{th}$ to $v = v_{th}$ after which the function monotonically decreases with v such that E tends to zero as v approaches infinity. E_{th} represents the maximum loss of energy to the crystal. As described by TF [80] the regime with $v < v_{th}$ represents a stable region, since any increase in velocity of the carrier from its steady state value causes energy losses to the crystal to increase over what is gained from the applied field, whereas, a decrease in velocity from its steady state velocity causes energy losses to decrease from what is gained from the applied field; hence, the carrier's velocity is restored to its original steady state value following any deviation. In contrast, $v > v_{th}$ represents an unstable region, since in this region, any increase in the velocity of the carrier from its steady state velocity causes the energy lost to the crystal to decrease; consequently, the carrier continues to gain energy from applied field.

For $\beta \geq 1$ the above equation exhibits very large oscillations beyond the threshold velocity; this fact has also emphasized by TF in [80] especially for $\beta \geq 10$; to ensure integration of Eq. 5.19 beyond threshold velocity, an approximation of Eq. 5.19 has been given in [80] as:

$$E = \frac{\alpha}{2v^2} \left(\frac{\beta}{\pi}\right)^{1/2} \frac{1}{\sinh\left(\frac{1}{2}\beta\right)} \int_0^{v/\sqrt{A}} x dx \int_{-\infty}^{+\infty} dk \frac{k}{|k|} \exp\left[-\frac{\beta k^2}{8A}\left(\frac{4B}{\beta^2} - A\right)\right]$$

$$\times \left(\left(e^{\frac{\beta}{2}} \right) e^{-\left(\frac{\beta}{2}\right)\left(x - \frac{k}{2} - \frac{1}{k^2}\right)^2} + \left(e^{-\frac{\beta}{2}} \right) e^{\beta/2\left(x - \frac{k}{2} - \frac{1}{k^2}\right)^2} \right)$$

(5.20)

where,

$$A = 1 + (1 - v_0^2/w_0^2) \left\{ v_0 \beta / \left[2 \sinh \left(\frac{1}{2} v_0 \beta \right) \right] - 1 \right\}$$

$$B = \beta \frac{w_0^2}{v_0^2} \left(\frac{v_0^2/w_0^2 - 1}{v_0} \tanh \left(\frac{1}{4} \beta v_0 \right) + \frac{1}{4} \beta \right)$$

The above equation is equivalent to Eq. 19 which allows integration beyond threshold velocity.

We observed that the above equation approximates the original equation accurately for all values of $\beta \geq 1$.

The above equations are expressed in units where $\hbar = \omega_{LO} = m = 1$ ($\omega_{LO} = LO$ phonon frequency and $m =$ mass of polaron)

Thornber and Feynman [80] have expressed the above equation in appropriate units as shown below:

$$F = (m/m_e)^{1/2} (\hbar \omega_L)^{3/2} E / 2.75 \quad [eV/\text{\AA}] \quad (5.21)$$

$$v_r = (m/m_e)^{1/2}(\hbar\omega_L)^{1/2}(v \times 0.418 \times 10^{16}) \quad [\text{\AA}/\text{sec}] \quad (5.22)$$

Feynman et al. [82] have computed the value of v_0 and w_0 for only 3 cases, namely:

$$\alpha = 3, 5 \text{ and } 7$$

To plot the above curves for any arbitrary value of coupling constant α , we apply the method of Ref. 83. In this paper, Feynman has defined v_0 and w_0 as a variational parameters in order to evaluate the ground state energy of polaron and its effective mass $\left(m^* \frac{v_0^2}{w_0^2}\right)$.

For determination of v_0 and w_0 , we need to minimize the polaron free energy expression of polaron at zero temperature defined in Ref. 82 which is recalled to be the following:

$$E = \frac{3}{4v}(v - w)^2 - \frac{\alpha v}{\sqrt{\pi}} \int_0^\infty \left[w^2 \tau + \frac{v^2 - w^2}{v} (1 - e^{-v\tau}) \right]^{-\frac{1}{2}} e^{-\tau} d\tau \quad (23)$$

To find the minima of E and the corresponding values of v_0 and w_0 , we performed a numerical evaluation which yields the values tabulated in Table 5.I. The minima of E is denoted by G and its value represents ground state energy of polaron. Table. 5.II shows all the parameters of all the materials used in this paper.

Table 5. I Material parameters for wurtzite crystals determined in this chapter.

		BN	ZnO	CdS	CdSe	ZnS	InN	SiC
LO phonon Frequency	ω_{LO}	1267.8	583.75	304.32	209.93	350	589.14	966.85
Average Fröhlich coupling const	α	0.3769	0.9328	0.6070	0.4838	0.6909	0.2067	0.3992
Angle at average value of coupling const	θ_{avg}	0.225π	0.231π	0.231π	0.238π	0.249π	0.233π	0.242π
Variational parameter	v_0	3.0389	3.1015	3.0639	3.0504	3.0734	3.0209	3.0412
Variational parameter	w_0	2.9529	2.8798	2.9231	2.9392	2.9122	2.9743	2.9500
Ground state energy of polaron	G	-0.3787	-0.9441	-0.6117	-0.4868	-0.697	-0.2072	-0.4012
Ratio of polaron mass to effective mass	m/m^*	1.0591	1.1599	1.0987	1.0771	1.1138	1.0316	1.0628
Mobility	$\mu \left(\frac{cm^2}{V-s} \right)$	2530.1	246.43	380.49	888.85	241.68	2560.6	502.58

Based on these TF predictions as well as the Fermi golden rule formulation described above, the results presented in Figure 2-3 give a comparison of the TF and the Fermi golden rule rates for BN, ZnO, CdS, CdSe, ZnS, InN, and SiC, respectively. These results show that the ratio of the TF rates to the Fermi golden rule scattering rates ranges from approximately 3 to 30 as shown in Figure 4 for BN, ZnO, CdS, CdSe, ZnS, InN, and SiC, respectively. These results show that for the strong carrier—optical-phonon interactions in these wurtzites leads to substantial corrections to the Fermi golden rule which is used widely in the study of carrier—optical-phonon interactions as well as in the design of electronic and optoelectronic devices based on these results. The correction curves of Fig. 4 provide the factors needed to correct the Fermi golden rule scattering rates for structures and devices based on these polar wurtzite materials.

Table 5. II Material properties of all semiconductors investigated in the current paper.

	BN^a	ZnO^b	CdS^c	$CdSe^c$	ZnS^d	InN^e	SiC^g
$\omega_{zL}(cm^{-1})$	1258	577.1	302.2	209	350	586	964
$\omega_z(cm^{-1})$	1006	380	234	165	270	447	788
$\omega_{\perp L}(cm^{-1})$	1281	592.1	307	211	350	593	970
$\omega_{\perp}(cm^{-1})$	1053	408.2	243	169	273	476	797
ϵ^∞	4.35	3.74	5.52	6.25	5.4	8.4	66
m^*/m_e	0.27	0.22	0.21	0.13	0.28	0.11 ^f	0.57 ^h

^a Reference 84

^e Reference 88

^b Reference 85

^f Reference 89

^c Reference 86

^g Reference 90

^d Reference 87

^h Reference 91

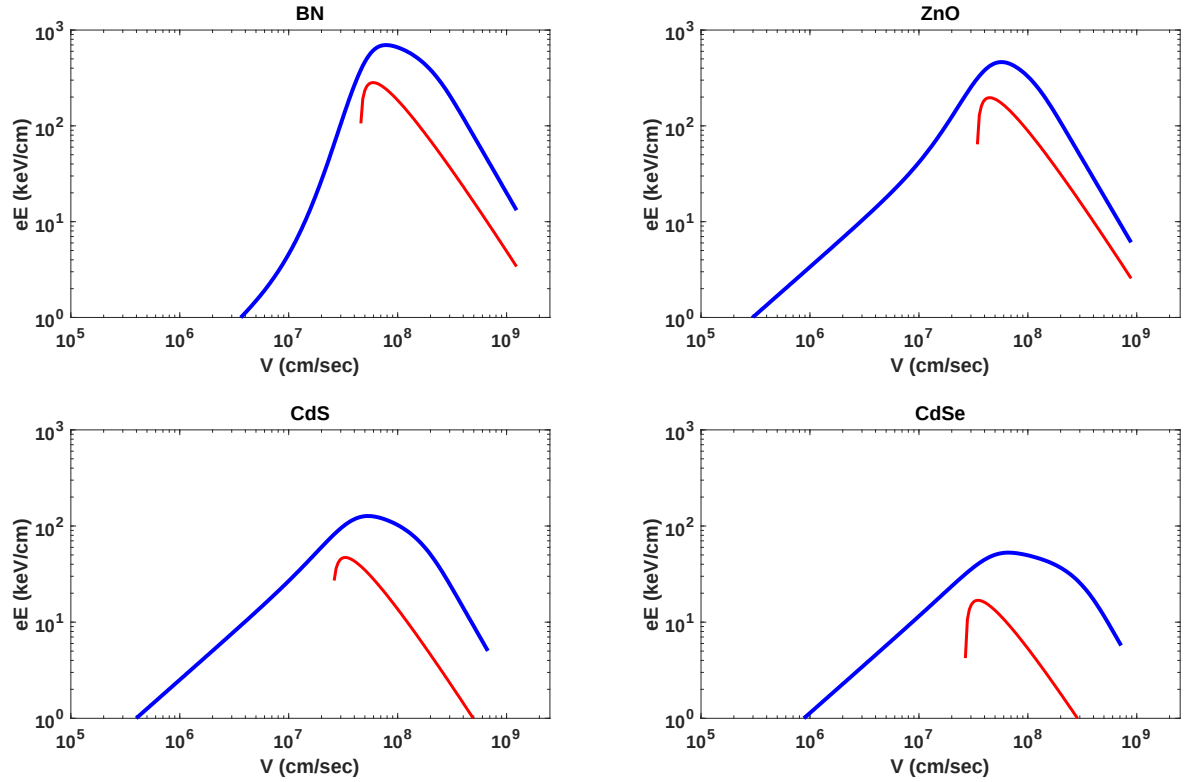


Fig. 5.2 Graphs showing Energy loss per unit distance versus electron velocity in TF (blue) and FGR (Red) regime for BN, ZnO, CdS and CdSe at temperature $T = 300K$.

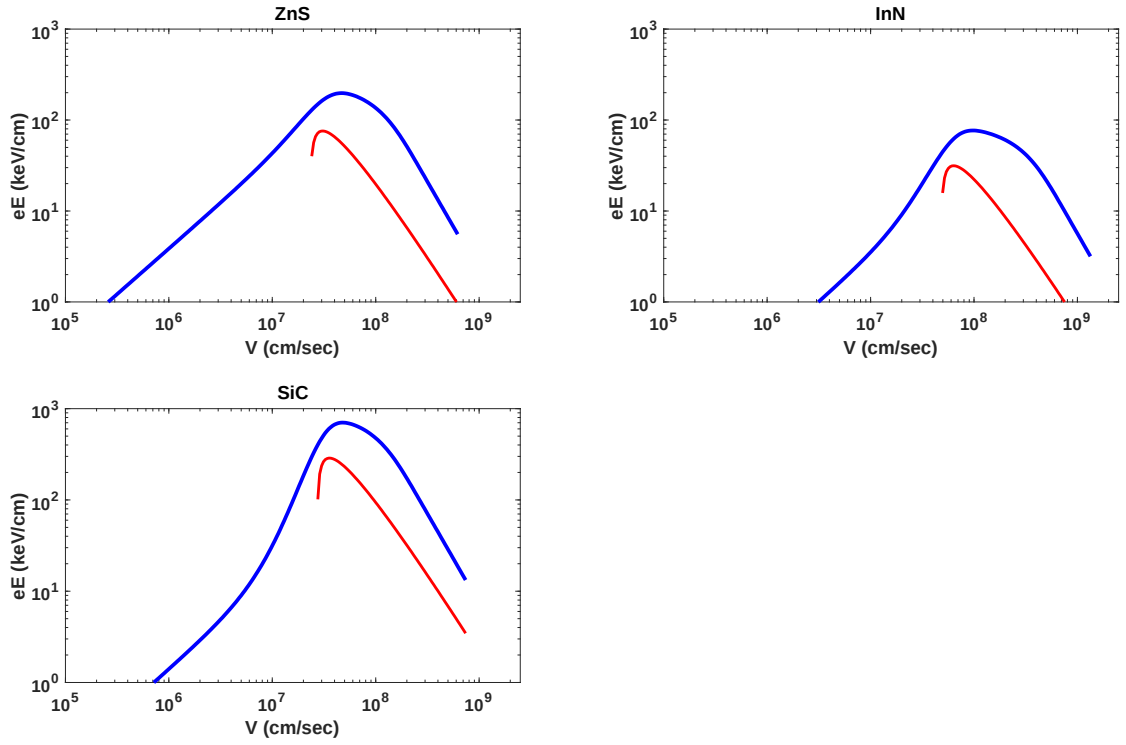


Fig. 5.3 Graphs showing Energy loss per unit distance versus electron velocity in TF (blue) and FGR (Red) regime for ZnS, InN and SiC at temperature $T = 300\text{K}$.

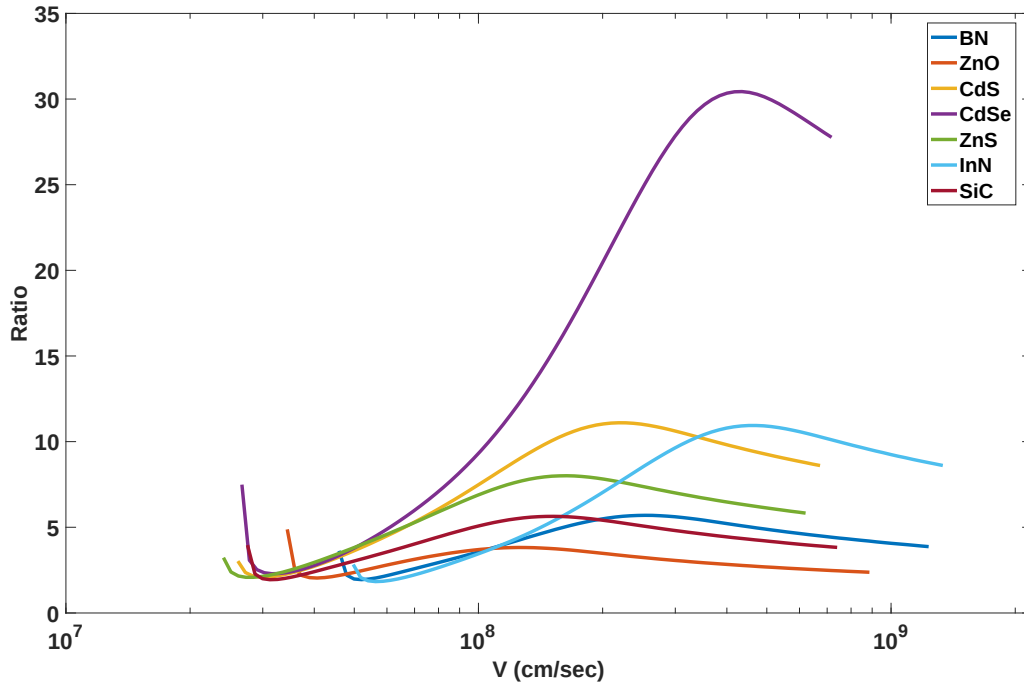


Fig. 5.4 Graph showing ratio of energy loss per unit distance in TF regime to FGR versus velocity at temperature $T = 300\text{K}$.

5.3 Conclusion

Optical phonon interactions play very important roles in a variety of electronic and optoelectronic devices based on polar wurtzite materials. Herein, it is shown that such wurtzite materials with Fröhlich coupling constants close to or greater than unity have carrier-optical-phonon rates that differ substantially from the common-used Fermi golden rule scattering rates. Using the non-perturbative path-integral approach of Thornber and Feynman it is shown that the commonly used perturbative approach of the Fermi golden rule does not give accurate scattering rates. As discussed herein, these corrections to the Fermi golden rule rates are due to the fact that for strong coupling constants, the first-order perturbative approach underlying the Fermi golden rule does not take into account the presence of many phonons interacting simultaneously with the carrier. These results show that the ratio of the TF rates to the Fermi golden rule scattering rates ranges from approximately 3 to 30 for the technologically important wurtzite materials of BN, ZnO, CdS, CdSe, ZnS, InN, and SiC.

Chapter 6

ELECTRON — OPTICAL-PHONON SCATTERING RATES IN CUBIC GROUP III-NITRIDE CRYSTALS : PATH-INTEGRAL CORRECTIONS TO FERMI GOLDEN RULE MATRIX ELEMENTS

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6.1 Introduction

The wurtzite phase of III-Nitride semiconductors have revolutionized the Light Emitting Diode (LED) industry in recent years because of direct bandgap ranging from 6.2 eV (AlN) to 1.95 eV (InN) at room temperature which covers the visible light spectrum and UV range. These LEDs are characterized by high brightness and high efficiency; for example, brightness of more than 10 cd has been achieved for blue, green and yellow InGaN LED [92]. A great variety of cubic and wurtzite structures have high technological interest [93-96].

III-Nitride semiconductors normally crystallize in wurtzite as well as cubic (zinc blende) structure, but for III-Nitrides the wurtzite phase is thermodynamically more stable structure at room temperature [97]. Phonon interactions have been modeled previously for wurtzite III-nitrides using the Fermi golden rule [7-8,79]. At present there are two major challenges for achieving higher efficiency with wurtzite III-Nitride semiconductors. First, the presence of spontaneous polarization causing a built in potential up to a few MV/cm [98]; this potential alters the potential inside the QW of active region of LEDs causing reduced efficiency of emission due to reduction

in overlap of electron and hole wavefunction (this phenomenon is better known as Quantum Stark Effect) [99]. Second, the crystal defects arising due to growth on lattice mismatched substrates like SiC, GaAs or sapphire which have been explored due to the high cost of GaN substrates [100]. The polarization field arises due to the growth of wurtzites as uniaxial crystals [101]. To mitigate the effects of the polarization field, growth along m-plane and a-plane have been considered but they have resulted in no significant improvement as compared with c-plane wurtzite. Recently, strong interests have been created in cubic (zinc blende) structures of III-Nitrides which offer the following advantages: a) absence of polarization fields, b) cleaving (0001) oriented zinc blende GaN along the vertical $\{110\}$ plane [99], c) theoretically the optical gain of cubic GaN might be higher than wurtzite phase [92], and d) normally off transistors [spontaneous polarization creates a 2DEG channel in AlGaIn/GaN transistors]. Liu and Bayram [102] have successfully produced high quality c-GaN through phase transition of MOVPE deposited GaN from hexagonal crystal to cubic via Si (100) nanopatterning. Also, motivated by the above advantages of cubic III-Nitrides, Novikov et al. [100] have shown great success in growing free standing cubic AlGaIn and GaN wafers using Plasma Assisted Molecular Beam Epitaxy (PA-MBE).

Over a wide range of temperature and crystal quality, the electron—polar-optical-phonon interaction is the dominant scattering mechanism affecting electron transport in polar semiconductors. In this paper we apply two different approaches to model the electron – polar optical phonon interaction, namely: (a) non-perturbative (path integral based) Thornber-Feynman model, and (b) Fermi’s golden rule - based on time dependent perturbative theory. We find that the generally-accepted Fermi-golden-rule rates are in error by nearly an order of magnitude.

6.2 Theory

First we consider the Thornber – Feynman model. This is a landmark model which uses the Fröhlich’s polaron model to describe the electron -optical phonon interaction using the path integral approach. The strength of electron – phonon coupling for a cubic crystal, which is an isotropic medium, is determined by the Fröhlich coupling constant as below:

$$\alpha = \frac{e^2}{\hbar} \left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0} \right) \left(\frac{m^*}{2\hbar\omega_{LO}} \right)^{\frac{1}{2}} \quad (6.1)$$

where, e is the elementary charge, ε_∞ and ε_0 are the high frequency and static dielectric constants, m^* is the electron effective mass and ω_{LO} is longitudinal optical phonon (LO phonon) frequency.

This model starts by describing the polaron model of an electron inside the polar semiconductor crystal which is based on the polarization of the lattice atoms in the vicinity of the electron which leads to modification in its energy and effective mass due to this interaction. The motion of an electron is thus accompanied with the associated distortion in the lattice [83]. Using variational method in [83], the expression of polaron energy is given as:

$$E = \frac{3}{4v} (v - w)^2 - \frac{\alpha v}{\sqrt{\pi}} \int_0^\infty \left[w^2 \tau + \frac{v^2 - w^2}{v} (1 - e^{-v\tau}) \right]^{-\frac{1}{2}} e^{-\tau} d\tau \quad (6.2)$$

v and w in the above equation are the variational parameters. The minimization of polaron energy as represented by the above equation yields the ground state energy, G , for a specific value of variational parameters v_0 and w_0 . This approach has been shown to yield moderate corrections to the Fermi golden rule for GaAs and AlAs and significant corrections for wurtzite III-nitrides

[81,103-104] but to our knowledge these techniques have not been applied previously to model corrections to the Fermi golden rule for the technologically important cubic III-nitrides, the subject of this paper.

In Ref. 80, Thornber and Feynman have explained that, in the materials with moderate to strong electron -phonon coupling - as determined by α in Eq (1) - the Fermi golden rule (which is based on perturbation theory) breaks down, as it considers subsequent LO phonon emission events as independent whereas in the case moderate to strong coupling the mean time between collisions is of the order of 10^{-15} sec [Ref. 80] and quantum interference between emitted phonons cannot be neglected and phonon emission events cannot be regarded as independent events.

Consequently, the specific problem of finding the expectation value of steady state velocity (v) of an electron is found for a given applied electric field, E . The kinetic energy gained by an electron (due to accelerating in the potential in the applied electric field) is exactly balanced by energy loss due to emission of LO phonon; hence, the rate of loss of energy per unit distance is equivalent to eE . Thornber and Feynman have thus expressed the result as:

$$E = \frac{\alpha}{2v^2} \left(\frac{\beta}{\pi}\right)^{1/2} \frac{1}{\sinh\left(\frac{1}{2}\beta\right)} \int_0^{v/\sqrt{A}} x dx \int_{-\infty}^{+\infty} dk \frac{k}{|k|} \exp\left[-\frac{\beta k^2}{8A} \left(\frac{4B}{\beta^2} - A\right)\right] \times \left(\left(e^{\frac{\beta}{2}}\right) e^{-\left(\frac{\beta}{2}\right)\left(x - \frac{k}{2} - \frac{1}{k^2}\right)^2} + \left(e^{-\frac{\beta}{2}}\right) e^{\beta/2\left(x - \frac{k}{2} - \frac{1}{k^2}\right)^2} \right) \quad (6.3)$$

where,

$$A = 1 + (1 - v_0^2/w_0^2) \left\{ v_0 \beta / \left[2 \sinh\left(\frac{1}{2} v_0 \beta\right) \right] - 1 \right\}$$

$$B = \beta \frac{w_0^2}{v_0^2} \left(\frac{v_0^2/w_0^2 - 1}{v_0} \tanh\left(\frac{1}{4}\beta v_0\right) + \frac{1}{4}\beta \right)$$

The above represents the relation between the electric field E required to balance the net loss of energy due to emission of phonons. In other words, it can be said that the above equation represents the electric field E required to maintain a steady state velocity (v) when the only way an electron can lose energy is by emission of phonons. In the above equation, α is the Fröhlich coupling constant, $\beta = \frac{\hbar\omega_{LO}}{KT}$ is the inverse temperature parameter, v_0 and w_0 are the variational parameters obtained by minimizing polaron energy as in Eq (2). E is a monotonically increasing function of v from $E = 0$ (at $v = 0$) to $E = E_{Th}$ (at $v = v_{Th}$). The region $0 < v < v_{Th}$ is the stable region in which E increases with v , as any deviation causing increase in electron velocity from its steady state value causes increase in energy loss to the lattice above which it gains energy from the applied electric field, whereas if the electron velocity decreases from its steady state value then the energy loss to lattice decreases causing it to gain energy from the applied field, hence, in both cases it returns to its steady state value. The region $v > v_{Th}$, is unstable region because E decreases with increase in v . In this region any increase in electron velocity above its steady state value causes the energy loss to the lattice to decrease, consequently it continues to gain energy from the applied field and hence if its kinetic energy becomes equal to the closest upper valley in the conduction band it can cause “runaway” – a well known high field transport condition in which the energy gained from the external field cannot be relaxed by the lattice. Furthermore, for $v > v_{Th}$ if the velocity of electron decreases then it causes an increase in the energy loss to lattice which leads to further decrease in velocity until it lands in the stable regime.

The Thornber – Feynman model allows us to determine the following parameters for the cubic III-Nitrides, which we are investigating in this paper:

v_{Th} : Threshold Velocity – the maximum velocity attainable under steady state regime.

E_{Th} : Maximum value of applied electric field beyond which electron pulls out of ‘polaron’ state and hence accelerates indefinitely (unless some other relaxation mechanisms like impurity scattering are present with higher threshold)

Runaway parameters: Here we investigate if a low field runaway is possible in cubic III-Nitrides, and compute the runaway length in appropriate cases.

Mobility: We will deduce mobility from the $E(v)$ curves by averaging $\mu = \frac{v}{E(v)}$ over the stable region of the curve.

Equation (6.3) is expressed in units where $\hbar = \omega_{LO} = m^* = 1$ (ω_{LO} = LO phonon frequency and m^* = effective mass of electron in the lattice). TF in [81] have expressed the above equation in appropriate units as below:

$$F = (m^*/m_e)^{\frac{1}{2}}(\hbar\omega_{LO})^{\frac{3}{2}}E/2.75 \quad [eV/\text{\AA}] \quad (6.4)$$

$$v_r = (m^*/m_e)^{\frac{1}{2}}(\hbar\omega_{LO})^{\frac{1}{2}}(v \times 0.418 \times 10^{16}) \quad [\text{\AA}/\text{sec}] \quad (6.5)$$

where, E and v are substituted in above equation from equation (6.3)

In the above equation m^* is the electron effective mass and m_e is the electron rest mass. The polaron effective mass is given as $m = m^* \frac{v_0^2}{w_0^2}$

Fermi's golden rule model:

In this model the energy relaxation time (for emission of LO phonon) for an isotropic medium can be expressed as below [1]:

$$\frac{1}{\tau^e} = \alpha \omega_{LO} \frac{1}{k} \sqrt{\frac{2m^* \omega_{LO}}{\hbar}} (N_q + 1) \ln \left[\frac{k + \sqrt{k^2 - \frac{2m^* \omega_{LO}}{\hbar}}}{k - \sqrt{k^2 - \frac{2m^* \omega_{LO}}{\hbar}}} \right] \quad (6.6)$$

In the above equation, k represents electron wave vector, $N_q = \frac{1}{\left(e^{\frac{\hbar \omega_{LO}}{KT}} - 1 \right)}$ is the phonon occupation number, m^* is the effective electron mass in the lattice.

Since, in the Fermi golden rule approach independent collisions are considered, we thus can say that electron emits a phonon of energy $\hbar \omega_{LO}$ after every τ^e seconds and hence travels a distance of $v \tau^e$, where $v = \sqrt{2m^* E_{el}}$ is the velocity of electron and E_{el} is the electron energy; this model is reported earlier in [81]. So, to allow comparison with Thornber – Feynman model, we can express energy loss per unit distance in the Fermi golden rule approach as:

$$eE = \frac{\hbar \omega_{LO}}{v \tau^e} \quad (6.7)$$

Now, we can simplify Equation (6) as below:

$$\frac{1}{\tau^e} = \sqrt{\frac{2m^*}{E_{el}}} \frac{e^2 \omega_{LO} (N_q + 1)}{\hbar} \left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0} \right) \ln \left[\sqrt{\frac{E_{el}}{\hbar \omega_{LO}}} - 1 + \sqrt{\frac{E_{el}}{\hbar \omega_{LO}}} \right] \quad (6.8)$$

The above simplification is performed in **Appendix B**.

It is to be noted that for all materials BN, AlN, GaN and InN $\beta = \frac{\hbar\omega_{LO}}{KT} > 1$ (see Table 6.II), hence, the physically realistic assumption that phonon emission dominates over phonon absorption has been made, and phonon absorption has not been taken into account in the above model. Phonon absorption becomes significant for temperatures above phonon energy.

6.3 Results and Discussion

For plotting the Thornber – Feynman curves we have used the polaron parameters for cubic BN, AlN, GaN and InN as reported in Table 6.I. The material parameters used for the cubic nitrides is tabulated in Table 6. II.

Fig. 6.1 presents plots showing energy lost per unit distance versus the electron velocity under both the Thornber – Feynman and the Fermi golden rule regimes. It is very conspicuous that the Fermi Golden rule underestimates the energy loss throughout the entire range of electron velocity under consideration. Fig .2 depicts the ratio of energy loss as predicted by the Thornber – Feynman model to the Fermi golden rule prediction values. These ratios range from 2 – 10 (for the velocity range under consideration) for BN, AlN and GaN whereas for InN it ranges from 2 – 14.

We report the threshold value of velocity, v_{Th} (which is the maximum attainable velocity in the stable regime on Thornber – Feynman curves) and E_{Th} (maximum value of electric field to ensure steady state velocity of electron) which corresponds to E_{max} on traditional experimentally obtained velocity – field curves used for determining mobility and other transport parameters) in Table 6. III. Zinc blende BN nitride though being an indirect band gap semiconductor is of limited importance in optoelectronics, but as seen from Table 6. III it exhibits highest threshold electric field of 1588 KV/cm as the phonon energy in BN nitride is 161.8 meV which is the highest of all

materials under consideration. Of all the materials, InN has the highest threshold velocity of 1.4×10^8 cm/sec (since, the Fröhlich coupling constant is least in InN).

Applying the approach in Ref. [81], we determine the possibility of low field runaway in cubic III-Nitrides. Fig. 6.3 shows the energy lost by electron per unit distance versus electron energy as determined under the Thornber – Feynman model. The vertical arrows represent the energy of the closest upper valley in the conduction band. Before proceeding further with this discussion on runaway we like to point out (for Fig. 6.3) that the Fröhlich coupling constant of BN is second highest (AlN has the highest = 0.7076, it is quite close to BN). The phonon energy in AlN is 111.2 meV but as shown in Table 6. II the polaron effective mass of BN is lower than AlN, and, therefore, we see that threshold is reached earlier in AlN as compared to BN. For all electron energies below the threshold for AlN the energy loss per unit distance is lower in BN as compared to AlN. As we have explained earlier, if for a given applied electric field the steady state solution of velocity falls in the “unstable” region then a slight increase in electron energy due to fluctuation would cause the energy loss to the lattice to decrease over the energy gained from the field. Under this condition the electron would continue to accelerate along the downward branch of the unstable region, and the magnitude of acceleration would continue to increase as the electron falls along the branch as the difference between applied field and the instantaneous field corresponding to electron energy increases. Finally, the electron appears in the next higher upper valley in the conduction band. Let us first consider the case of AlN, let the applied field be 626 KeV/cm, this field corresponds to electron energy $\approx 1\text{eV}$ (unstable region) and $\approx 0.2\text{ eV}$ (for stable region). If the injected electron energy in the AlN sample is more than 1 eV (say 2.1 eV) then it will be acted upon by a force equal to difference between applied field and the field corresponding to its instantaneous energy along the way downward in the unstable branch. If we assume maximum force acting on the electron (equal to difference between applied field and field corresponding to

closest upper valley = 270 KeV/cm) we achieve a “runway” in a distance of $L_r^{AlN} > 30 \text{ nm}$. We also observe that for InN - which has smallest Fröhlich coupling constant - there is a very broad region near the peak, if we carry out similar analysis we find the runaway length to be $L_r^{InN} > 909 \text{ nm}$ which is significantly large and practically precludes runaway as other scattering mechanisms would come into play along the journey of the electron. Also, for BN we find $L_r^{BN} > 18 \mu\text{m}$ making runaway unlikely. But in AlN the runaway is highly likely.

The mobility values as deduced from the Thornber – Feynman model are reported in Table

6. IV. As expected, InN with lowest Fröhlich coupling constant has a mobility of $6541 \frac{\text{cm}^2}{\text{V-sec}}$ whereas AlN with highest coupling constant has a low mobility of $438 \frac{\text{cm}^2}{\text{V-sec}}$.

6.4 Conclusion

In this paper we have established that Fermi’s Golden rule in cubic III-Nitrides - which have high Fröhlich coupling constant (close to 1) - underestimates the energy lost by an electron to the lattice under an applied electric field. We have estimated threshold values of velocity, electric field and mobility under the Thornber – Feynman regime and most importantly we have determined the corrections to E-v relationship when Fermi’s Golden rule is applied to it.

Table 6.I Polaron parameters for cubic III-Nitrides in units where $\hbar = \omega_{LO} = m^* = 1$ (These parameters are used to integrate Eq (6.3) and finally we plot the curves using equation (6.4) and (6.5) respectively)

	Fröhlich coupling constant	v_0	w_0	Ground state energy (G)	Ratio of polaron mass to lattice effective mass $\frac{m}{m^*}$
BN	0.5648	3.0592	2.9286	- 0.5689	1.0912
AlN	0.7076	3.0753	2.9100	-0.7140	1.1169
GaN	0.3527	3.0362	2.9559	-0.3543	1.0551
InN	0.1703	3.0172	2.9789	-0.1707	1.0259

Table 6.II. Material parameters for cubic III-Nitrides

	BN	AlN	GaN	InN
$\omega_{LO}(cm^{-1})$	1305 ^a	897 ^d	735.5 ^g	588.7 ^g
ϵ_∞	4.5 ^b	4.25 ^e	5.35 ^g	8.4 ^g
m^*	0.64 ^c	0.33 ^f	0.15 ^g	0.054 ^g
β	6.26	4.30	3.53	2.82

^a Reference 105

^d Reference 108

^g Reference 111

^b Reference 106

^e Reference 109

^c Reference 107

^f Reference 110

Table 6. III Threshold values of electron velocity and applied electric field. (These values are analogous to Vmax and Emax on velocity - field curves for scattering limited to LO phonons)

	BN		AlN		GaN		InN	
	TF	FGR	TF	FGR	TF	FGR	TF	FGR
$v_{Th}(x 10^7 \text{ cm/s})$	5.14	4	5.9	4.4	8.7	6.2	14	8.8
$E_{Th}(\text{KV/cm})$	1588	674	780	345.3	204.8	86.17	43.84	17.88

Table 6. IV Mobility of cubic III-Nitride at T = 300 K obtained in non-perturbative TF model and compared with FGR first order results.

	Mobility $\left(\frac{cm^2}{V-sec}\right)$ (in TF)	Mobility $\left(\frac{cm^2}{V-sec}\right)$ (in FGR)
BN	838	830
AlN	438	1660
GaN	1412	16,937
InN	6541	408,990

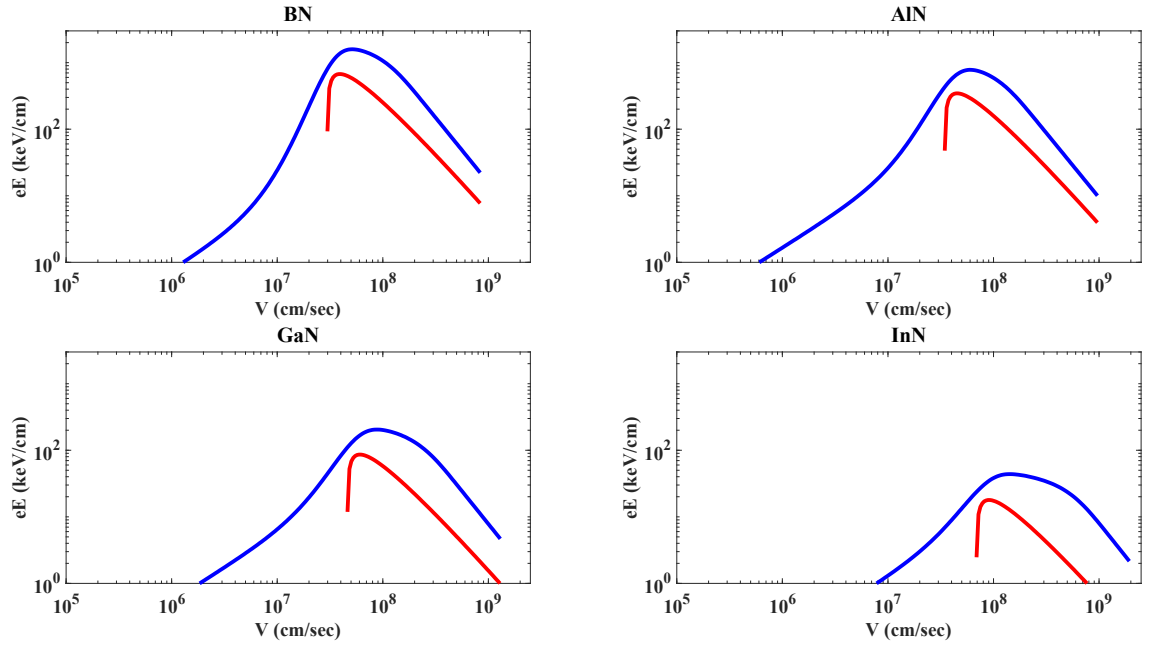


Fig. 6.1 Graph showing energy loss per unit distance versus electron velocity at T =300K for cubic-BN, AlN, GaN and InN respectively. Blue line represents Thorner -Feynman curve and Red line shows Fermi's golden rule model.

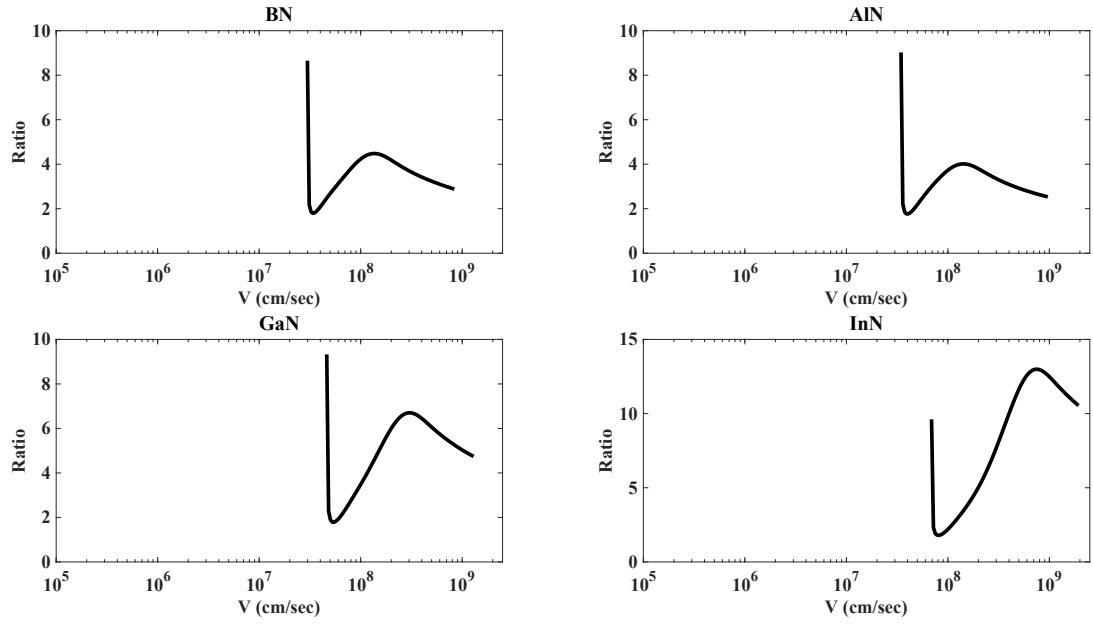


Fig. 6.2 Plots showing the ratio of energy loss predicted by Thornber -Feynman model to those predicted by the Fermi golden rule model for cubic-BN, AlN, GaN and InN respectively.

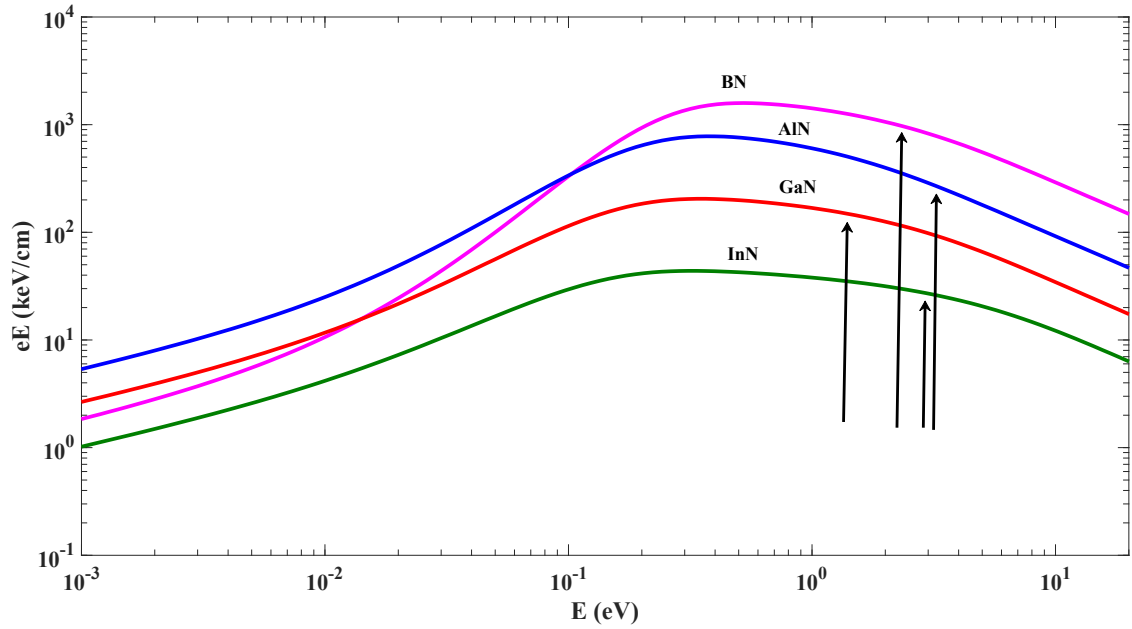


Fig. 6.3 Plot showing energy loss per unit distance versus polaron energy at $T = 300$ K (Thornber - Feynman model). The energy of the closest upper valley is indicated by vertical arrows.

Chapter 7

ELECTRIC FIELD – VELOCITY RELATION FOR STRONGLY COUPLED FRÖHLICH POLARON IN EMERGING 2D MATERIALS

[Submitted for publication]

7.1 Introduction

Graphene's zero band gap is a major limitation in its application to electronic devices despite its zero effective mass and high mobility ($\sim 10^4 \text{ cm}^2/\text{V} - \text{sec}$) [112-113]. Accordingly, there has been extensive research on potential two dimensional alternatives, including, TMDc (Transition Metal Dichalcogenides). These TMDc are of the form MX_2 where M is a transition metal and X is a chalcogen, namely, S, Se or Te. Previous studies on carrier transport have been done on monolayer group IV chalcogenides for $M = \text{Mo}, \text{W}$ and have concluded that carrier – longitudinal acoustic (LA) phonon scattering is the dominant mechanism limiting mobility at room temperature between the range $180 - 800 \text{ cm}^2/\text{V} - \text{sec}$ [114-116].

On the other hand, group IV chalcogenides with $M = \text{Hf}$ and Zr have been predicted to have high carrier mobility at room temperature [117-118]. It should be noted that, the carrier – longitudinal optical (LO) phonon coupling will become the dominant scattering mechanism at room temperature and above if the carrier – LO phonon coupling increases, which is defined by the dimensionless Fröhlich coupling constant α [1,119]:

$$\alpha = \frac{e^2}{\hbar} \left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0} \right) \left(\frac{m_b}{2\hbar\omega_{LO}} \right)^{1/2} \quad (7.1)$$

where, m_b is the effective electron mass in the conduction band, ϵ_∞ and ϵ_0 are the (in-plane) high frequency and static dielectric constant and $\hbar\omega_{LO}$ is the zone-center LO phonon energy, and e is the electronic charge. Previous studies [114,116,120] on MoX_2 ($X \equiv S, Se \text{ and } Te$) and WX_2 ($X \equiv S, Se \text{ and } Te$) have studied the electron – LO phonon interaction within the purview of Fermi's Golden Rule (FGR) which is based on first order perturbation theory. The electron coupling to LO phonons in MoX_2 and WX_2 may be modeled using the Fermi Golden Rule since the Fröhlich coupling constant α is small compared to unity: for MoX_2 ($X \equiv S, Se \text{ and } Te$), 0.0048, 0.03 and 0.07, respectively, and for WSe_2 , 0.0157. On the other hand, the values of α for HfX_2 ($X \equiv S \text{ and } Se$) are 0.7875 and 0.5879, and for ZrX_2 ($X \equiv S \text{ and } Se$), 0.8495 and 0.6471 which indicate that the electrons couple more strongly to LO phonons in the these materials. For such materials with strong coupling as indicated by high α , the FGR model breaks down which assumes that collisions of electrons with LO phonons are independent; that is, they are sufficiently separated in time so that there is no quantum interference between the collisions and a further assumption is that the electron interacts with only one phonon at a time. As an example, it was first noted in the context of 3D materials [80] that, for the materials with LO phonon energy in the range 50 – 100 meV the mean free time between collisions (based on perturbative treatment) becomes as small as 2×10^{-15} sec which is further reduced at high temperatures where phonon absorption becomes significant. Consequently, in our previous work on 3D wurtzite [104] and cubic materials [121] we investigated the energy loss per unit distance (electric field) versus electron velocity in high alpha materials in the purview of non-perturbative path integral formalism by Thornber and Feynman (TF) [80] and the FGR model and found that the FGR model underestimates the energy lost by the electron as a result of the Fröhlich interaction, as it neglects the situation of many phonons interacting with the electron simultaneously and the quantum interferences between the emitted phonons in successive collisions; in such situations the

scattering events cannot be separated in time. The correction factors for the energy loss for the FGR was about an order of magnitude and higher for materials with α in the range 0.21 – 0.93 for wurtzite and 0.1 – 0.7 for cubic materials. In this paper we apply Thornber – Feynman path integral formalism for HfX_2 ($X \equiv S, Se$) and ZrX_2 ($X \equiv S, Se$) and determine the electric field vs velocity relation and also determine other transport parameters such as peak velocity, peak electric field, mobility and effective polaron mass.

7.2 Theory

An electron in any polar material interacts strongly with the neighboring lattice causing it to distort, as a result the electron is surrounded with a cloud of phonons, a state referred to as “polaron”. This distorted lattice state moves along with the electron in the lattice [82,83]. The electron in the lattice experiences increased apparent effective mass and undergoes change in its eigen energy states. Further, if the local distortion in the lattice due to the LO phonon interaction is assumed to be absent or weak the electron moves like a free particle with energy, $E_k = \frac{\hbar^2 k^2}{2m_b}$ (assuming parabolic conduction band). 3D bulk polarons have been studied in detail in the past [83]. In [83] Feynman modelled the electron interaction with LO phonon in the purview of Fröhlich model where the LO phonon perturbation Hamiltonian is given as:

$$H = \sum_q (C_q a_q e^{iq \cdot r} + C_q^* a_q^\dagger e^{-iq \cdot r}) \quad (7.2)$$

where,

$$C_q = \left(-i \frac{\hbar \omega_{LO}}{q} \right) \left(\frac{\hbar}{2m_b \omega_{LO}} \right)^{\frac{1}{4}} \left(\frac{4\pi\alpha}{V} \right)^{1/2}$$

In the above equation, q is the LO phonon wave vector and V is the volume of the material. The LO phonon frequency ω_{LO} is assumed to be dispersion less and taken as the zone center frequency. Feynman applied the path integral method to eliminate the lattice coordinates to find the upper bound on the ground state eigen energy of the polaron (see Eqs. 31 & 33 in [83]). For the present 2D case we use the 2D scaled Hamiltonian of Eq (7.2) [122], such that:

$$C_q = \frac{C}{\sqrt{q}} = -i\hbar\omega \left(\frac{\sqrt{2}\pi\alpha}{Aq} \right)^{1/2} \left(\frac{\hbar}{m_b\omega} \right)^{1/4} \quad (7.3)$$

where, $\mathbf{q}$ and $\mathbf{r}$ are 2D vectors and A is the area of the material. The ground state energy of this 2D Fröhlich polaron is obtained by minimizing the following expression with respect to the variational parameters v and w [122,123]:

$$G = \frac{(v-w)^2}{2v} - \frac{\alpha}{2} \left(\frac{\pi}{2} \right)^{\frac{1}{2}} \int_0^\infty dt \frac{e^{-t}}{\sqrt{\frac{w^2}{2v^2}t + \frac{v^2-w^2}{2v^3}(1-e^{-vt})}} \quad (7.4)$$

Further, the mass of polaron becomes:

$$m^* = m_b \frac{v_0^2}{w_0^2} \quad (7.5)$$

where, v_0 and w_0 are obtained after minimizing G in Eq. (7.4). We plot variation of v_0 and w_0 as a function of α in Fig. 7.1(a) and variation of ratio of polaron mass to effective mass of electron, $\frac{m^*}{m_b}$ in Fig. 7.1(b).

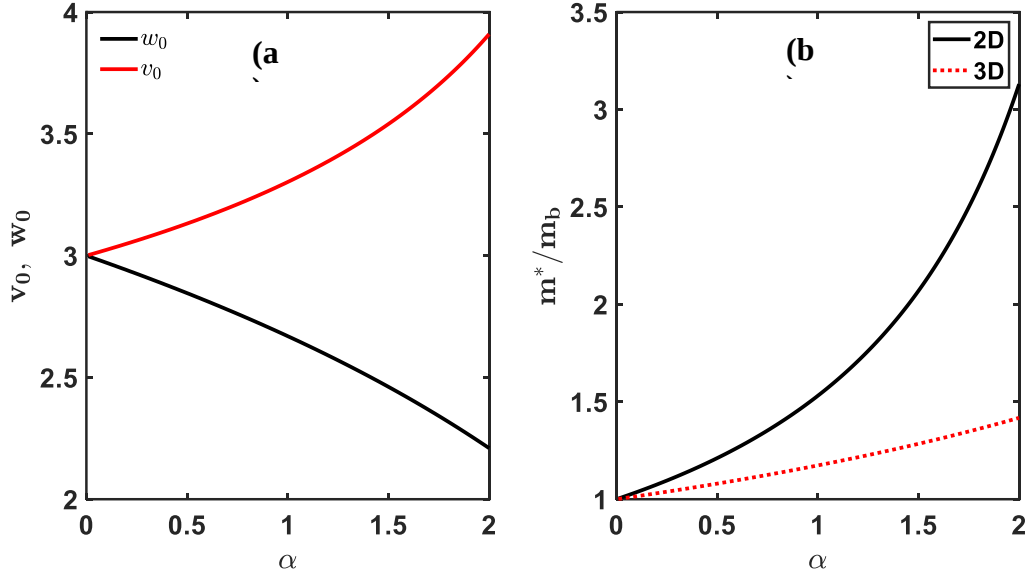


Fig. 7.1 (a) Variational parameters v_0 and w_0 obtained after minimizing Eq. 7.4 shown for different Fröhlich coupling constant α , (b) Ratio of polaron mass to effective mass of electron in conduction band for various α for 2D and 3D respectively.

From Fig 7.1(a) and (b), it is evident that in weak coupling limit $v_0 \rightarrow w_0$ and $m^* \rightarrow m_b$. It is to be noted that there exists a definite scaling relation between 3D and 2D polaron properties which has been derived in [124] and is reproduced below:

$$\frac{m_{2D}^*(\alpha)}{(m_b)_{2D}} = \frac{m_{3D}^*\left(\frac{3\pi}{4}\alpha\right)}{(m_b)_{3D}} \quad (7.5.1)$$

$$Z_{2D}(\alpha; \omega) = Z_{3D}\left(\frac{3\pi}{4}\alpha; \omega\right) \quad (7.5.2)$$

$$\mu_{2D}(\alpha) = \mu_{3D}\left(\frac{3\pi}{4}\alpha\right) \quad (7.5.3)$$

It can be seen from Eq. 7.5.1 and in Fig. 7.1(b) dotted line that for the same value of α the 2D polaron is heavier as compared to a 3D polaron. Further, Eq. 7.5.2 and 7.5.3 suggest that the apparent impedance experienced by the polaron and its mobility in 2D can be computed from the 3D expression as in Refs. 80 and 82 with the substitution $\alpha \rightarrow \frac{3\pi}{4}\alpha$.

7.3 Electric Field – Velocity relation

In [80], motivated by finding the peak energy loss of the electron to the lattice due to interaction with LO phonon, Thornber – Feynman approached the entire problem by finding the expectation value of the steady – state velocity obtained by the electron when subjected to a one - dimensional electric field E . The general expression (expressed in Feynman units $\hbar = m_b = \omega_q = 1$) which preserves the physics of the problem is given below:

$$\mathbf{E} = \int_{-\infty}^{\infty} d\xi \sum_q |C_q|^2 \mathbf{q} \frac{\cos(\omega_q \xi)}{\sin\left(\frac{1}{2}\beta\omega_q\right)} e^{-\mathbf{q}\cdot\mathbf{v}(\xi+i\beta/2)} e^{-k^2 \bar{K}_{\beta'}(\xi)} \quad (7.6)$$

where, $\beta = 1/k_B T$ in Feynman units ($\beta = \hbar\omega_{LO}/k_B T$ in SI units), $\mathbf{v}$ is the steady state velocity of electron and $K_{\beta'}(\xi)$ is a an expression which depends on impedance of the electron and oscillator distribution, $K_{\beta'}(\xi) = D(\xi + i\beta/2)/2$ [80,82] is given as below:

$$\bar{K}_{\beta'}(\xi) = \frac{1}{2} \frac{w_0^2}{v_0^2} \left[\left(\frac{v_0^2 - w_0^2}{w_0^2 v_0} \right) \times \frac{\cosh\left(\frac{1}{2}\beta v_0\right) - \cos(v_0 \xi)}{\sinh\left(\frac{1}{2}\beta v_0\right)} + \frac{\xi^2}{\beta} + \frac{\beta}{4} \right]$$

In the above expression of $K_{\beta'}(\xi)$, the v_0 and w_0 are as given in Fig. 7.1(a). In the Feynman model it is assumed that the phonon model of the lattice consists of a single frequency. It should be noted that $\mathbf{E}$ in Eq. (6) represents $e\mathbf{E}$, and the Eq. (7.6) should be interpreted as electric field necessary to balance the loss of energy by the electron to the lattice as a result of LO phonon interaction while maintaining a steady state velocity $\mathbf{v}$.

We need to scale Eq. (7.6) for the 2D case, we start by expanding $\cos(v_0\xi)$ to the second power in the expression of $\bar{K}_{\beta'}(\xi)$, such that $\cos(v_0\xi) = 1 - \frac{v_0^2\xi^2}{2}$, consequently we can write (the simplification is shown in Appendix C.I) :

$$\bar{K}_{\beta'}(\xi) = \frac{B_0}{2\beta} + \frac{A_0\xi^2}{2\beta}$$

where,

$$A_0 = \left[\left(\frac{v_0^2 - w_0^2}{v_0^2} \right) \times \left\{ \frac{v_0\beta}{2\sinh\left(\frac{1}{2}\beta v_0\right)} - 1 \right\} + 1 \right] \quad (7.7)$$

$$B_0 = \frac{\beta w_0^2}{v_0^2} \left[\left(\frac{v_0^2 - w_0^2}{w_0^2 v_0} \right) \times \tanh\left(\frac{1}{4}\beta v_0\right) + \frac{\beta}{4} \right]$$

Now, substituting for $\bar{K}_{\beta'}(\xi)$ from Eq. (7.7) in Eq. (7.6), we get (the simplification is shown in Appendix C.II):

$$E = \frac{\alpha}{4 \sinh\left(\frac{1}{2}\beta\right)} \cdot \sqrt{\frac{\beta}{\pi}} \cdot \frac{1}{A_0} \int_0^{2\pi} d\phi \cos(\phi) \int_0^\infty dk \frac{q}{|q|} \exp\left(-\frac{\beta q^2}{8A_0} \left[\frac{4B_0}{\beta^2} - A_0\right]\right) \\ \times \left(e^{\frac{-\beta}{2}} \exp\left(\frac{-\beta}{2} \left(\frac{\cos(\phi)v}{\sqrt{A_0}} - \frac{q}{2} + \frac{1}{q}\right)^2\right) + e^{\frac{\beta}{2}} \exp\left(\frac{-\beta}{2} \left(\frac{\cos(\phi)v}{\sqrt{A_0}} - \frac{q}{2} - \frac{1}{q}\right)^2\right) \right) \quad (7.8)$$

The expression in Eq. (7.8) is the final expression for the energy lost per unit distance ($\mathbf{eE}$), in Feynman units, for an electron interacting with LO phonons in a 2D polar medium with a steady state velocity $\mathbf{v}$.

Now, we derive the Fermi's golden rule based model to compare it with the above expression obtained in the purview of non-perturbative treatment. The scattering rate of phonons for an electron for a transition from a state $|\mathbf{k}\rangle$ to $|\mathbf{k}'\rangle$ is given as:

$$\frac{1}{\tau^{e,a}} = \frac{2\pi}{\hbar} |M_q|^2 \delta(E(\mathbf{k}') - E(\mathbf{k}) \pm \hbar\omega_{LO}) \quad (7.9a)$$

where, the upper '+' sign in the parenthesis indicates emission and the lower '-' for absorption respectively. M_q is the electron – phonon coupling matrix element defined by [1]:

$$M_q = \left\langle \mathbf{k}', N_q + \frac{1}{2} \pm \frac{1}{2} \right| H_{Fr} \left| \mathbf{k}, N_q + \frac{1}{2} \pm \frac{1}{2} \right\rangle \quad (7.9b)$$

In Eq. 7.9(b), $N_q = 1/(\exp(\frac{\hbar\omega_{LO}}{kBT}) - 1)$ is the phonon occupation number. It is to be noted that during emission of phonons the electron – phonon state changes from $|\mathbf{k}, N_q\rangle$ to $|\mathbf{k}', N_q + 1\rangle$ and during absorption it changes from $|\mathbf{k}, N_q\rangle$ to $|\mathbf{k}', N_q - 1\rangle$. We consider the electrons to be strictly two dimensional, so the wavefunction can be written as:

$$|\mathbf{k}\rangle = \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{\sqrt{A}} \quad (7.10)$$

Evaluating the equation 7.9(a), we get:

$$\frac{1}{\tau^{e,a}} = \alpha\omega_{LO} \sqrt{\frac{\hbar\omega_{LO}}{\mathcal{E}}} \left(N_q + \frac{1}{2} \pm \frac{1}{2}\right) \int_{q_{min}}^{q_{max}} \frac{dq}{q} \frac{1}{\sqrt{1 - \frac{\hbar^2}{2m_b\mathcal{E}} \left(\frac{q}{2} \pm \frac{m_b\omega_{LO}}{q\hbar}\right)^2}} \quad (7.11)$$

where, $\mathcal{E} = \frac{\hbar^2 k^2}{2m_b}$ is the kinetic energy of the electron in the conduction band and q_{min} and q_{max} are the limits determined for emission and absorption as follows:

Emission:

$$q_{min} = \frac{\sqrt{2m_b}}{\hbar} (\sqrt{\mathcal{E}} - \sqrt{\mathcal{E} - \hbar\omega_{LO}})$$

$$q_{max} = \frac{\sqrt{2m_b}}{\hbar} (\sqrt{\mathcal{E}} + \sqrt{\mathcal{E} - \hbar\omega_{LO}})$$
(7.12)

Absorption:

$$q_{min} = \frac{\sqrt{2m_b}}{\hbar} (-\sqrt{\mathcal{E}} + \sqrt{\mathcal{E} + \hbar\omega_{LO}})$$

$$q_{max} = \frac{\sqrt{2m_b}}{\hbar} (\sqrt{\mathcal{E}} + \sqrt{\mathcal{E} + \hbar\omega_{LO}})$$
(7.13)

From Eq. (7.11) it follows that an electron loses an energy $\hbar\omega_{LO}$ when it travels a distance $v\tau^e$ and similarly it gains $\hbar\omega_{LO}$ when it travels $v\tau^a$ so the net loss in energy per unit distance in the FGR regime is given by [81]:

$$E = \frac{\hbar\omega_{LO}}{v} \left(\frac{1}{\tau^e} - \frac{1}{\tau^a} \right)$$
(7.14)

Also, from Eq. (7.12) it is clear that the condition for emission is $\mathcal{E} \geq \hbar\omega_{LO}$ because the limits must be a real positive number which represents the phonon wave vector. So, the FGR predicts that no loss of energy takes place unless the electron energy is greater than or equal to the LO phonon energy.

7.4 Results and Discussion

We first plot in Fig. 7.2 the phonon emission and absorption rates in FGR regime as obtained in Eq. (7.11), we observe that for all the four materials the phonon emission rate is $\sim 2.1 - 3.7$ times higher than the phonon absorption rate at room temperature (actual values tabulated in Table. 7.I), unlike 3D materials where the emission rate is about an order of magnitude or higher [1]. Thus, the phonon absorption rate cannot be neglected here at room temperature and have been duly accounted for in Eq. (14) to model energy loss per unit distance. From Fig. 2 and Table I, we see that the mean time between the emission ranges from $\sim 0.9 \times 10^{-14} - 1.7 \times 10^{-14}$ sec whereas, the FGR is valid only when the electron phonon interaction time scale $t \gg \frac{2}{\omega_{LO}}$ [1,104] which lies in the range $\sim 3.9 \times 10^{-14} - 6.9 \times 10^{-14}$ sec. It is evident that the mean time between phonon emissions is even smaller than the minimum interaction time required for the validity of the FGR.

Now we plot Thornber – Feynman curves as obtained in Eq. (7.8) after converting from Feynman units and compare them with FGR curves as obtained in Eq. (7.11). We see that the TF curves exhibit a monotonically increasing relation between eE and velocity until a threshold velocity v_{th} which corresponds to peak energy loss, say eE_{th} . This region with increasing slope is the stable region as any increase in the velocity (due to fluctuation) causes energy loss to the lattice to increase and hence the velocity decreases until the total loss is balanced by the energy gained from the electric field, alternatively, if the velocity decreases then the loss to the lattice is reduced

below what the electron gains energy from the external field due to this net gain of energy the velocity increases until the loss to lattice is balanced by the gain from the field. Similarly, the region with negative slope in the TF curve is the unstable region as any increase in the velocity is accompanied by a decrease in the energy loss to the lattice consequently the electron gains a net energy and continues to accelerate indefinitely unless there are some other scattering mechanisms with higher thresholds.

We have tabulated the peak energy loss and the threshold velocity for all the materials in Table . II. We can see that ZrS_2 with Fröhlich coupling constant $\alpha = 0.85$ has maximum energy loss and $HfSe_2$ with $\alpha = 0.59$ has minimum peak energy loss, the peak energy loss should increase with α as it indicates strong interaction with LO phonons. However, we also expect that a higher α will increase the apparent mass as in Fig . 7.1(b) this increase causes reduction in the threshold velocity because near the threshold region $\frac{1}{2} m_b \left(\frac{v_0}{w_0} \right)^2 v_{th}^2 \approx \hbar \omega_{LO}$ [80] and hence as depicted in Table 7.II we observe that with increasing α the threshold velocity is reduced . However, the ratio of peak energy loss as predicted by TF to FGR peak increases with decrease in β . We see that for HfS_2 with $\beta = 1.28$ has the ratio 2.4 whereas for $ZrSe_2$ which has lowest $\beta = 0.74$ at room temperature of all the four materials has a ratio of 3.5, this is because a lower β implies higher phonon occupation number N_q and since the energy loss to lattice in TF formalism duly takes care of interferences between emitted phonons predicts a higher energy loss as compared to TF which treats phonon emissions independent of each other. Finally, we deduce the mobility, μ_{TF} using the $E(v)$ curves in Fig. 7.3 by finding averaging $\frac{dv}{dE(v)}$ in the stable region [121], we have depicted

them in Table 7.III. It is seen that $ZrSe_2$ has the highest mobility $449.1 \frac{cm^2}{V-s}$ of all the materials followed by $HfSe_2$ whose mobility is $239.78 \frac{cm^2}{V-s}$.

Table 7.I. Comparison of min interaction limit with actual phonon mean free time

	$t_{min} = \frac{2}{\omega_{LO}} \text{ (x } 10^{-14} \text{ sec)}$	Average mean time between phonon emission (x 10^{-14} sec)
HfS_2	3.97	0.97
$HfSe_2$	5.2	1.6
ZrS_2	4.1	0.92
$ZrSe_2$	6.9	1.7

Table 7.II Comparison of computed TF and FGR parameters

	TF		FGR		$\frac{E_{th}^{TF}}{E_{th}^{FGR}}$	$\beta = \frac{\hbar\omega_{LO}}{k_B T}$	α	$\left(\frac{\mu_{TF}}{V-s} \right)$
	E_{th} (KV/cm)	v_{th} (x 10^7 cm)	E_{th} (KV/cm)	v_{th} (x 10^7 cm)				
HfS_2	476	3.0	196.7	2.2	2.42	1.28	0.7875	90.76
$HfSe_2$	246.6	4.0	87.7	2.3	2.81	0.98	0.5879	239.78
ZrS_2	576.7	2.5	231.8	1.93	2.49	1.24	0.8495	58.32
$ZrSe_2$	252	3.8	72	1.77	3.5	0.74	0.7371	449.1

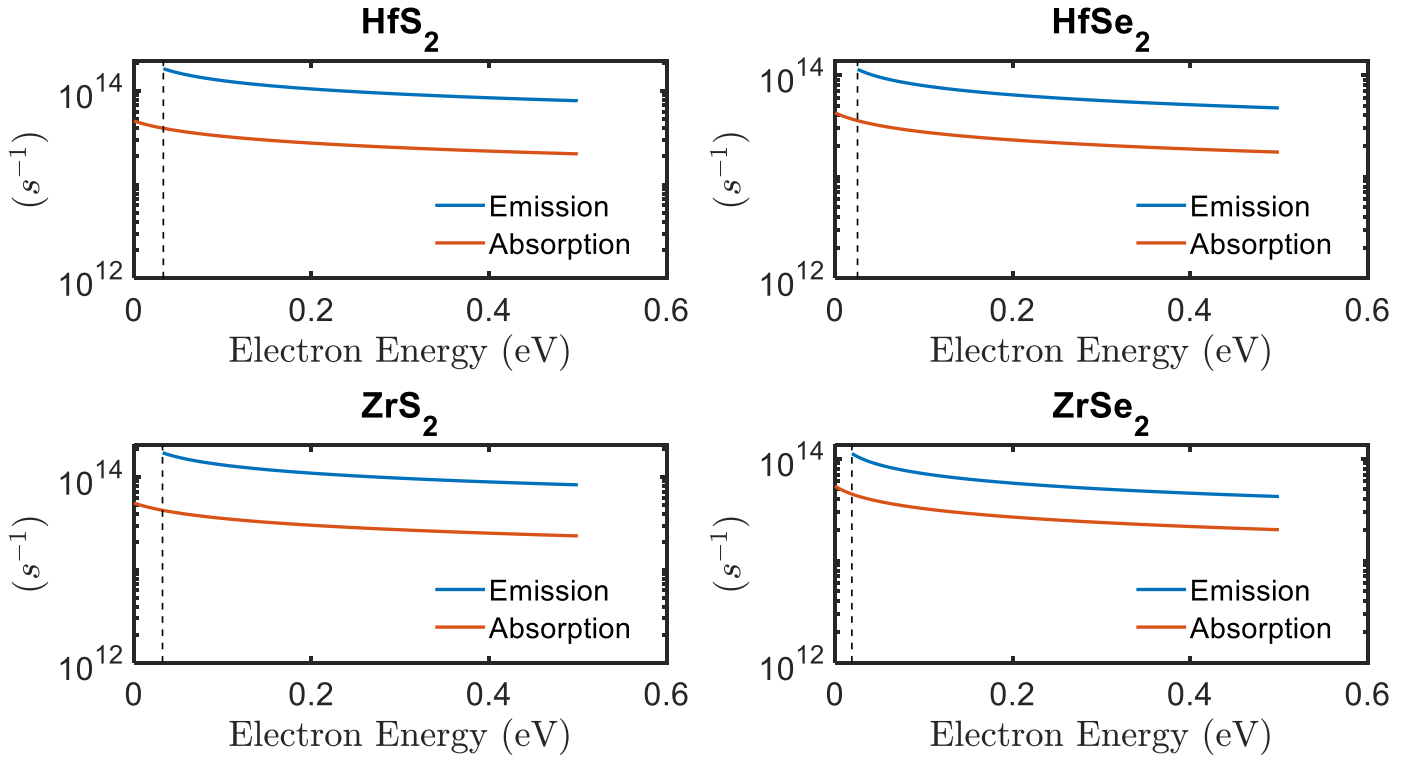


Fig. 7.2 Phonon emission and absorption rates obtained under Fermi's Golden Rule formalism. The dashed line indicates the emission threshold $\hbar\omega_{LO}$ for different materials whose values are given in Table 7.III.

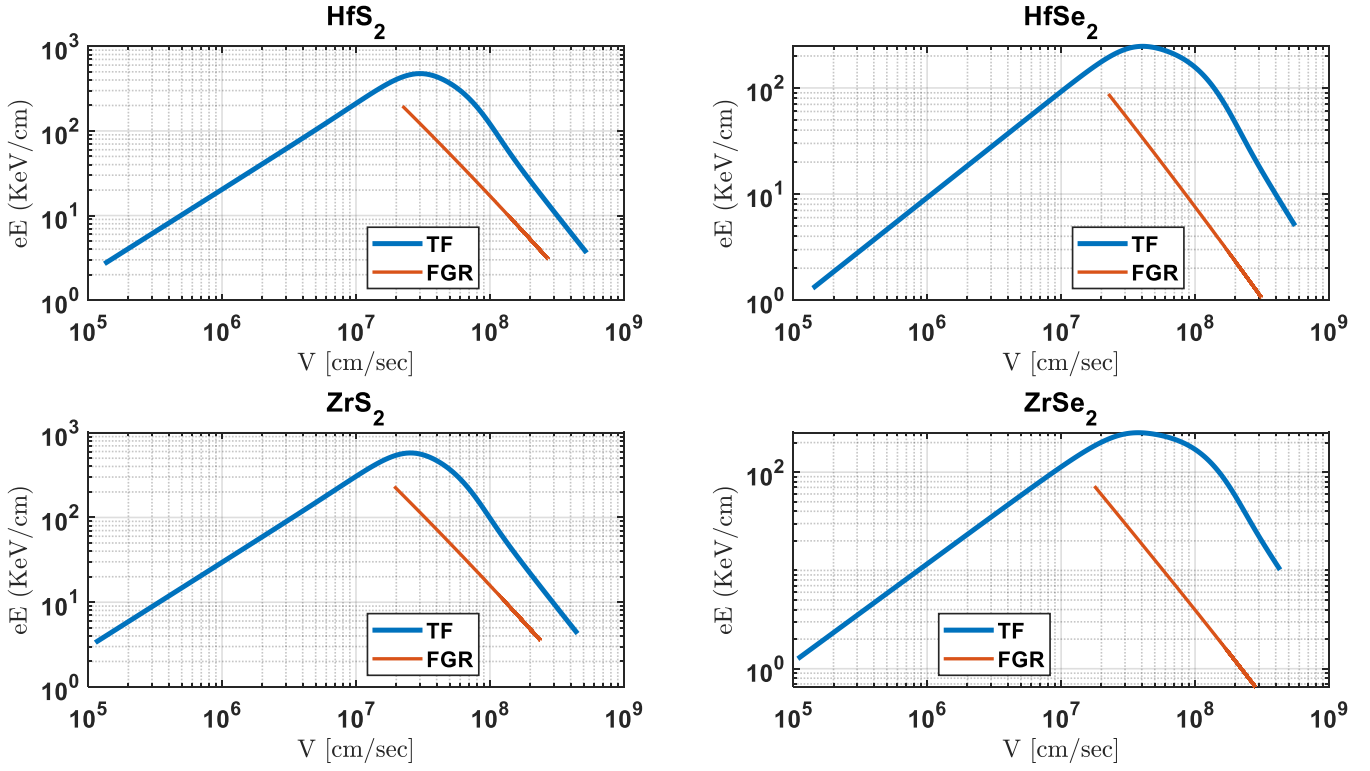


Fig. 7.3 Comparison of Thornber – Feynman vs. FGR based electric field versus velocity curves for electron.

Table 7.III Material parameters used in calculation for 3D materials

	$\omega_{LO}(cm^{-1})$	m_b	ϵ_∞	ϵ_0
HfS_2	267.6 ^a	0.24 ^a	10.2 ^b	53.6 ^b
$HfSe_2$	205 ^a	0.18 ^a	13.9 ^b	83 ^b
ZrS_2	260.2 ^a	0.31 ^a	11.2 ^b	66.7 ^b
$ZrSe_2$	153.7 ^a	0.22 ^a	15.76 ^c	84.59 ^c

^aReference [125]

^bReference [126]

^cReference [127]

7.5 Conclusions

In this paper we have evaluated energy lost per unit distance (electric field) versus velocity of electrons for 2D materials with strong carrier - LO phonon interactions within the purview of Thornber – Feynman formalism applied to 2D Fröhlich polaron. We demonstrated that Fermi's Golden Rule based scattering rate cannot be applied to these materials and it underestimates the energy loss by the electron to the lattice. We find the energy loss rates are underestimated by the FGR by about an order of magnitude for the materials considered with the largest carrier – LO phonon coupling constants. Finally, out of all four materials $ZrSe_2$ has the highest mobility 449.1

$\frac{cm^2}{V-s}$ at room temperature.

Chapter 8

ROLE OF CONFINED OPTICAL PHONONS IN EXCITON GENERATION IN SPHERICAL QUANTUM DOTS

[Submitted to MDPI, Materials]

8.1 Introduction

The discrete energy levels in quantum dots (QDs) due to confinement of carriers in three dimensions makes them attractive in quantum information processing for applications such as single photon source [128] and entangled photon source [129]. The excitonic excitations in a single QD form a basis for a two level system to be implemented as a qubit in quantum computing applications [130]. The qubit states can be manipulated by optical excitations using laser sources [131]. In the recent past, numerous studies have been done with III-V-based self-assembled QDs for qubit state preparation [132-136]. These self-assembled quantum dots are nanoscale islands of a smaller bandgap material embedded in the matrix of larger bandgap material with a smaller mismatch in their elastic properties [137]. The discrete energy states in the QD are subjected to interactions with phonon modes leading to dephasing [136-138]. However, the phonon modes also lead to the creation of excitons and such schemes have been studied extensively taking into account bulk acoustic phonon modes [132-136]. However in the past, experimental observation was made on the role of longitudinal optical (LO) phonon assisted exciton generation in InGaAs/GaAs based QD [139]; it was observed that the exciton generation was caused due to emission of LO phonon of frequencies which is equal to near-zone center (in GaAs) value . In III-V based QDs the polar optical modes are significantly modified as a result of confinement [1,13-15]. The modified polar optical modes are (a) confined LO modes, and (b) surface optical (SO) modes. In this paper we

investigate the role of confined LO phonon modes using the dielectric continuum model [1,3,142] in the creation of excitons when subjected to a continuous optical energy from an incident laser.

8.2 Description of confined phonon modes

Let the quantum dot of radius R with a dielectric constant $\varepsilon_1(\omega)$ be embedded in the barrier material with dielectric constant $\varepsilon_2(\omega)$. The polar optical phonon modes inside and outside the quantum dot produce macroscopic polarization $\mathbf{P}$, due to which the associated electric displacement vector $\mathbf{D}$, the electric field $\mathbf{E}$, and the Fröhlich potential, Φ , in each medium are related as follows [1,3,142]:

$$\mathbf{D} = \varepsilon \mathbf{E} = \mathbf{E} + 4\pi \mathbf{P} \quad ((8.1))$$

$$\mathbf{E} = -\nabla \Phi \quad ((8.2))$$

$$\nabla \cdot \mathbf{D} = 0 \quad ((8.3))$$

In equation (8.1), $\varepsilon(\omega)$ obeys the Lyddane-Sach-Teller relation as below:

$$\varepsilon_{1,2}(\omega) = \varepsilon_\infty \frac{\omega^2 - \omega_{LO_{1,2}}^2}{\omega^2 - \omega_{TO_{1,2}}^2} \quad ((4))$$

where, ω_{LO} and ω_{TO} are the zone center LO and TO phonon frequency and ε_∞ is the high frequency dielectric constant. The divergence of the displacement vector $\mathbf{D}$ vanishes in Eq. (8.3) because it is assumed that no free charge exists inside the material. Now, from Eq. (8.1) – (8.3), we get the following relation in each medium:

$$\varepsilon(\omega) \nabla^2 \Phi(\mathbf{r}) = 0 \quad ((8.5))$$

There are two possible solutions which satisfy Eq. (8.4): (a) confined LO phonon modes, which corresponds to $\varepsilon(\omega) = 0$ (b) surface optical modes, which corresponds to $\nabla^2\Phi(\mathbf{r}) = 0$. For the confined LO modes, the phonon frequency satisfies $\varepsilon(\omega) = 0$, which results in $\omega = \omega_{LO}$ and the eigenfunction corresponding to potential $\Phi(\mathbf{r})$ can be expressed in spherical coordinates (with origin at the center of the quantum dot) after expanding in terms of complete set of orthogonal functions $j_l(qr)Y_l^m(\theta, \varphi)$ as follows:

$$\Phi(r) = \sum_{l,m} \sum_q B_q j_l(qr) Y_l^m(\theta, \varphi) \quad (8.6)$$

In Eq. (8.6), $j_l(qr)$ with $l = 0, 1, 2, 3 \dots$ represents the spherical Bessel functions of order l , $Y_l^m(\theta, \varphi)$ represents the spherical harmonics such that $-l \leq m \leq l$ and $B_q = \sqrt{\frac{2}{R^3}} \cdot \frac{1}{j_{l+1}(qR)}$ is the normalization constant. Using Eq. (8.6), after imposing the electrostatic boundary conditions: (a) continuity of the potential Φ at the interface (b) continuity of normal component of the displacement vector $\mathbf{D}$, we see that the potential Φ must vanish at the interface $r = R$; hence, equating Eq. (8.6) to zero we get:

$$j_l(qR) = 0. \quad (8.7)$$

Eq. (8.7) leads to the following solution:

$$q_n = \frac{x_{n,l}}{R} \quad ((8.8)$$

where, $x_{n,l}$ is the n^{th} zero of the l^{th} order spherical Bessel function. Eq. (8.8) is very significant as it describes the effect of dimensional confinement on phonon wave vector which becomes discrete as opposed to being continuous in the case of bulk material. Finally, the Fröhlich potential

as given in Eq. (8.6) can be represented in second quantized form after duly considering quantization of amplitudes of the ionic pair of the material as below [140]:

$$\Phi(\mathbf{r}) = \sum_{l,m} \sum_n f_{lm}(q_n) [\hat{a}_{l,m}(q_n) j_l(q_n r) Y_l^m(\theta, \varphi) + H.C.] \quad (8.9)$$

where,

$$f_{lm}(q_n) = \left(\frac{2\pi\hbar\omega_{LO} B_q^2}{q_n^2} \right)^{1/2} \left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0} \right)^{1/2}$$

In Eq. (8.9), H.C. represents Hermitian conjugate and $\hat{a}_{l,m}$ is the phonon annihilation operator.

8.3 Confined LO phonon – exciton interaction

We assume a parabolic confinement potential for the exciton in the ground state [136], so that the net charge density can be written as:

$$\rho(\mathbf{r}) = -e \left(\frac{e^{-r^2/a_e^2}}{\pi^{3/2} a_e^3} - \frac{e^{-r^2/a_h^2}}{\pi^{3/2} a_h^3} \right) \quad (8.10)$$

where, a_e and a_h are the electron and hole confinement length such that $a_h = a_e/1.15$ in GaAs taking into account the heavier hole effective mass than that for the electron [136]. The charge density in Eq. (8.10) represents a hole in the heavy hole valence band and electron in the conduction band both with anti-parallel spins. Now, the confined LO phonon mode interacts with the exciton due to the Fröhlich potential Φ , so the interaction Hamiltonian can be expressed as:

$$H_{Fr} = \int d^3r \rho(\mathbf{r}) \Phi(\mathbf{r}) |2\rangle\langle 2| \quad (8.11)$$

Substituting, for $\Phi(\mathbf{r})$ from Eq. (8.9) in Eq. (8.11) we get:

$$H_{Fr} = \sum_{l,m} \sum_n \left\{ \hat{a}_{l,m}(q_n) f_{lm}(q_n) \int d^3r j_l(q_n r) Y_l^m(\theta, \varphi) \rho(\mathbf{r}) + H.C \right\} |2\rangle\langle 2| \quad (8.12)$$

Now since,

$$\int_{\varphi=0}^{\varphi=2\pi} \int_{\theta=0}^{\theta=\pi} Y_l^m(\theta, \varphi) \sin \theta d\theta d\varphi = \sqrt{4\pi} \delta_{l,0} \delta_{m,0} \quad (8.13)$$

Hence, only confined LO phonon modes corresponding to $l = 0, m = 0$ mode contribute to the exciton – phonon interaction as represented by the interaction Hamiltonian in Eq. (8.12).

Substituting the results of Eq. (8.13) in Eq. (8.12), we get:

$$H_{Fr} = \sum_q \{ \hat{a}_{0,0}(q) v(q) + H.C \} |2\rangle \langle 2| \quad (8.14)$$

where,

$$v(q) = f_{00}(q) M(q) \quad (8.15)$$

and where, $f_{00} \equiv f_{l=0,m=0}$ and $M(q) = -\frac{2e}{\pi} \int_{r=0}^{r=R} r^2 dr \frac{\sin(qr)}{qr} \left(\frac{e^{-r^2/a_e^2}}{a_e^3} - \frac{e^{-r^2/a_h^2}}{a_h^3} \right)$

Recalling that for $l = 0$, $j_{l=0}(q_n R) = \frac{\sin(q_n R)}{q_n R}$ so from Eq. (8.8) we get:

$$q_n = \frac{x_{n,0}}{R} = \frac{n\pi}{R} \quad (8.16)$$

The discrete phonon dispersion relation obtained for the $l = 0$ mode is plotted below in Fig . 8.1, note that the curve in the dashed line corresponds to the bulk GaAs dispersion relation.

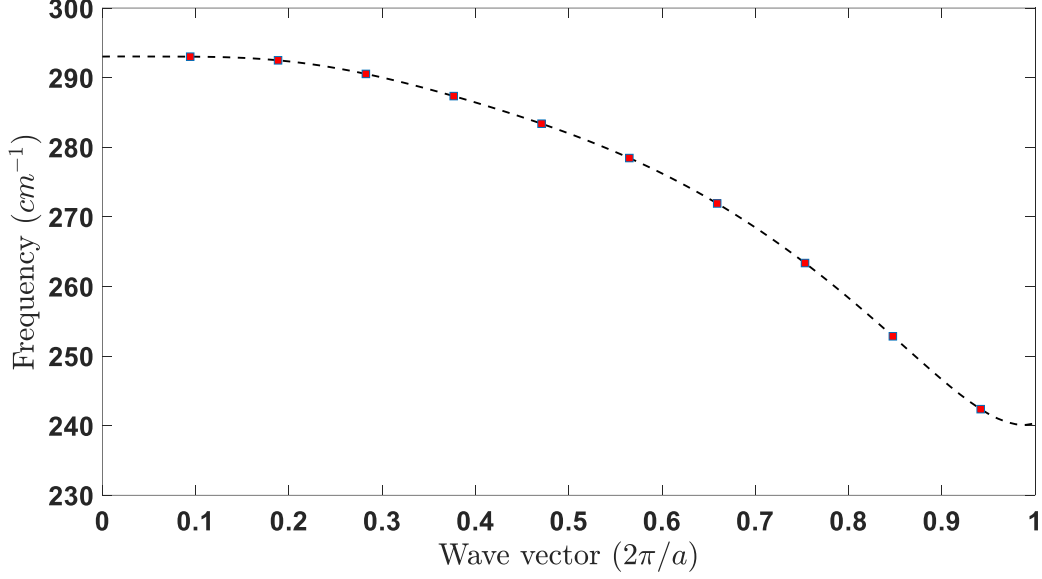


Fig. 8.1 Dispersion relation in GaAs, the dashed lines show for bulk case and the square dots represents the 10 modes obtained for GaAs QD of radius 3 nm. In the above figure, $a = 5.65 \text{ \AA}$ lattice constant for GaAs.

8.4 Confined LO-phonon-assisted exciton creation for QD interacting with classical light

For implementation of a QD as a qubit, the QD is subjected to a coherent laser for excitation of the excitonic state. In this section we investigate the confine LO-phonon-assisted creation of excitons in the presence of laser light which can be modelled a classical light. Here, we consider the QD as the two level system (TLS) consisting of a ground state $|1\rangle$ with a zero reference energy and the excitonic state represented by $|2\rangle$, let the separation of energy $\hbar\omega_0$. The theory of a TLS interacting with classical light is well known [143]; however, we provide a brief summary. Later in the section, we will introduce the Fröhlich Hamiltonian as a perturbation which triggers the phonon-assisted process. The interacting electric field with the QD can be expressed as:

$$\mathbf{E}(t) = E_0 \hat{\mathbf{e}} \cos(\omega t) \quad (8.17)$$

It is assumed that the interacting electric field has a wavelength much greater than the dimensions of QD so the spatial dependence in Eq. (8.17) has been dropped. Let the difference between the laser frequency ω and the excitonic resonance frequency ω_0 be defined as: detuning, $\Delta = \omega - \omega_0$. The interaction of this classical field with the TLS can be expressed as a dipole in the dipole approximation as follows:

$$H_{dot-field} = -\mathbf{d} \cdot \mathbf{E} \quad (8.18)$$

where, $\mathbf{d}$ is the dipole operator associated with the TLS. The total Hamiltonian which is the summation of TLS bare Hamiltonian $\hbar\omega_0|2\rangle\langle 2|$ and $H_{dot-field}$ can be expressed in the Rotating Wave Approximation (RWA) as follows:

$$H_{RWA} = \hbar \begin{bmatrix} 0 & \Omega/2 \\ \Omega/2 & -\Delta \end{bmatrix} \quad (8.19)$$

where, Ω is the Rabi frequency defined as:

$$\Omega = -\frac{2\langle 1|\hat{\mathbf{e}} \cdot \mathbf{d}|2\rangle E_0}{\hbar} \quad (8.20)$$

The Hamiltonian H_{RWA} as in Eq. (8.19) is expressed in the uncoupled bare TLS basis comprising $|1\rangle$ and $|2\rangle$. The eigen states H_{RWA} are referred to as Dressed basis (which is light + TLS coupled basis) are given as below:

$$|\psi\rangle_+ = \sin \theta |1\rangle + \cos \theta |2\rangle \quad (8.21)$$

$$|\psi\rangle_- = \cos \theta |1\rangle - \sin \theta |2\rangle \quad (8.22)$$

where, θ is the Stückelberg angle defined as:

$$\tan 2\theta = -\frac{\Omega}{\Delta} \quad (8.23)$$

The eigen value of energy of states in Eq. (8.21) and (8.22) is given as:

$$E_{\pm} = -\frac{\hbar\Delta}{2} \pm \frac{\hbar\sqrt{\Delta^2 + \Omega^2}}{2} = -\frac{\hbar\Delta}{2} \pm \frac{\hbar\Omega}{2} \quad (8.24)$$

where, Ω^Δ is the generalized Rabi frequency. It is clear from Eq. (8.24) that the separation of levels in TLS has now become $\hbar\Omega^\Delta$ which was originally $\hbar\omega_0$ in the absence of light. From Eqs. (8.21), (8.22) and (8.23) it is seen that if the detuning is positive such that $\Delta \gg \Omega$ then $\theta \approx \pi/2$, so that $|\psi_-\rangle \approx |2\rangle$ and $|\psi_+\rangle \approx |1\rangle$ in such condition phonon-assisted transitions can happen if the exciton decays with an emission of confined LO phonon with energy $\hbar\omega_n = \hbar\Omega^\Delta$. And since, ω_n is of discrete nature (frequency of confined mode corresponding to wave vector q_n as depicted in Fig. 8.1) we can have such phonon-assisted transitions for specific values of detuning at which the energy gap between the dressed state becomes equal to the individual discrete phonon mode of energy $\hbar\omega_n$ (see Fig. 8.2). We proceed to find such probability per unit time using Fermi's Golden Rule in the next paragraph.

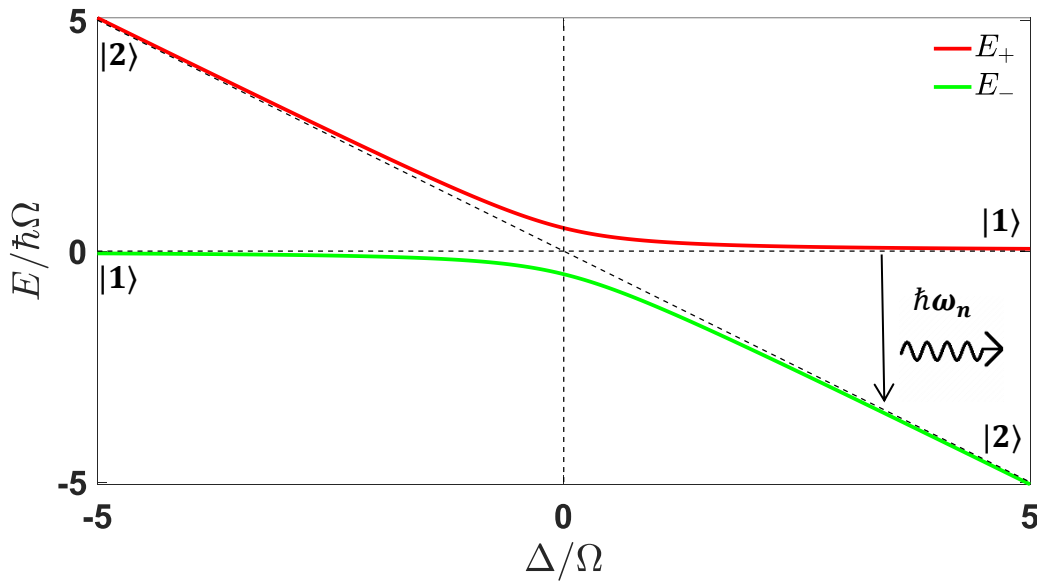


Fig. 8.2 The dressed state energy variation with Δ/Ω is shown. The slant dashed line represents the energy of $|2\rangle$ state with value $-\hbar\Delta$ and the horizontal dashed line represents the energy of state $|1\rangle$, when there is no coupling between the bare QD states and the classical light. The solid vertical arrow represents transition from the upper dressed state to lower dressed state when detuning is sufficiently high so that $|\psi_-\rangle \approx |2\rangle$ and $|\psi_+\rangle \approx |1\rangle$ and the emitted phonon has the energy $\hbar\Omega^\Delta = \hbar\omega_n$ (where ω_n is the frequency of confined LO mode of mode n).

Using Eqs. (8.14), (8.21) and (8.22) we can express the exciton – phonon interaction (perturbation) Hamiltonian in the dressed basis as follows:

$$H_{Fr} = \sum_{q,v} (v(q)\hat{a}_{00}(q) + H.C) (\sin^2\theta |\psi_-\rangle\langle\psi_-| + \cos^2\theta |\psi_+\rangle\langle\psi_+| + \frac{1}{2}\sin 2\theta |\psi_-\rangle\langle\psi_+| + \frac{1}{2}\sin 2\theta |\psi_+\rangle\langle\psi_-|) \quad (8.23)$$

The transition involves change of state from $|\psi_+, N_q\rangle$ to $|\psi_-, N_q + 1\rangle$, where $N_q = \frac{1}{\exp(\hbar\omega_n/k_{BT})-1}$ is the phonon occupation number of phonon mode with energy $\hbar\omega_n$. The transition probability per unit time (or the exciton creation rate) given by:

$$\begin{aligned} \frac{1}{\tau} &= \frac{2\pi}{\hbar} \sum_q |M_q|^2 \delta(E_- - E_+ + \hbar\omega_n) \\ \text{where,} \quad M_q &= \langle N_q + 1, \psi_- | H_{Fr} | \psi_+, N_q \rangle \\ \text{so,} \quad M_q &= \frac{1}{2} \sin 2\theta v(q)^* (N_q + 1)^{1/2} \end{aligned} \quad (8.24)$$

Substituting, $E_- - E_+ = -\hbar\Omega^\Delta$ in Eq. (8.24), we get:

$$\frac{1}{\tau} = \frac{\pi}{2} \sin^2 2\theta J_{ph}(\Omega_n^\Delta) \quad (8.25)$$

where, $J_{ph}(\Omega^\Delta)$ is the phonon spectral density as shown below:

$$J_{ph}(\Omega_n^\Delta) = \frac{1}{\hbar^2} \sum_n |v(q)|^2 \delta(\Omega^\Delta - \omega_n) (N_q + 1) \quad (8.26)$$

To evaluate the phonon spectral density (which is now discrete, hence the generalized Rabi frequency is labelled by subscript n), we substitute $q_n = n\pi/R$ in Eq. (8.15) and obtain the now discrete version of $M(q)$ as M_n by performing a numerical integration over r , we write the phonon spectral density as below in Eq. (8.27):

$$J_{ph}(\Omega_n^\Delta) = \frac{4\pi e^2 \omega_{LO}}{\hbar R} \left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0} \right) (N_q + 1) \sum_n \frac{M_n \delta_{\omega_n, \Omega_n^\Delta}}{\omega_n} \quad (8.27)$$

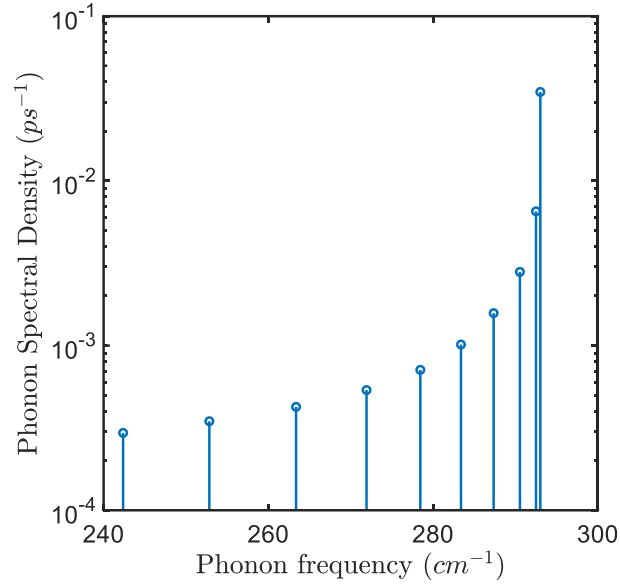


Fig. 8.3 Confined LO mode phonon spectral density for a GaAs quantum dot of radius, $R = 3$ nm at $T = 1$ K. The discrete spectrum depicts the strength corresponding to each phonon mode contained in the 1st Brillouin zone (total 10 modes), with $n = 1$ having the highest magnitude and is located near the zone center.

In Fig. 8.3, we plot the discrete phonon spectral density corresponding to all 10 modes (whose discrete dispersion is shown in Fig. 8.1). As we can see that corresponding to $n = 1$ mode which is near the zone center of the Brillouin zone has the highest magnitude of 0.035 ps^{-1} of all the modes.

8.5 Results and discussion

Eq. (8.25) represents transition rate from the lower dressed state to upper dressed state, the energy gap between the two dressed state is $\hbar\Omega^\Delta = \hbar\sqrt{\Omega^2 + \Delta^2}$ (the energy gap depends on applied field strength and detuning). When this gap is equal to one of the confined LO phonon mode then phonon-assisted transitions can result in transitions. And as pointed out in the previous section, that the final state will have more excitonic character if $\frac{\Delta}{\Omega} \gg 1$ when $\Delta > 0$ (see Fig. 2). Such exciton occupancy in the final state (lower dressed state) is given by:

$$|\langle 2|\psi\rangle_-|^2 = \sin^2 \theta = \frac{1}{2} \left\{ 1 + \frac{\Delta^2}{\Delta^2 + \Omega^2} \right\} \quad (8.28)$$

However, In Ref. 144, it was demonstrated that the final exciton occupation taking into account temperature is given by Eq. (8.29) and is plotted in Fig. 3(b):

$$C_{exc} = \frac{1}{2} \left\{ 1 + \frac{\Delta}{\Omega^\Delta} \tanh \left(\frac{\hbar\Omega^\Delta}{2k_B T} \right) \right\} \quad (8.29)$$

Now, as we can see from Eq. (8.25) that the transition rate is directly proportional to the strength of phonon spectral density, but, from Fig. 3 we see that except for $n = 1$ mode the contribution to such transition is negligible. So, for the $n = 1$ mode, Eq. (8.25) can be written as in Eq. (8.30) for which we plot in Fig. 4 the transition rate as a function of Δ/Ω :

$$\frac{1}{\tau} = \frac{\pi}{2} \frac{1}{\sqrt{(\Delta/\Omega)^2 + 1}} J_{ph}(\omega_1) \quad (8.30)$$

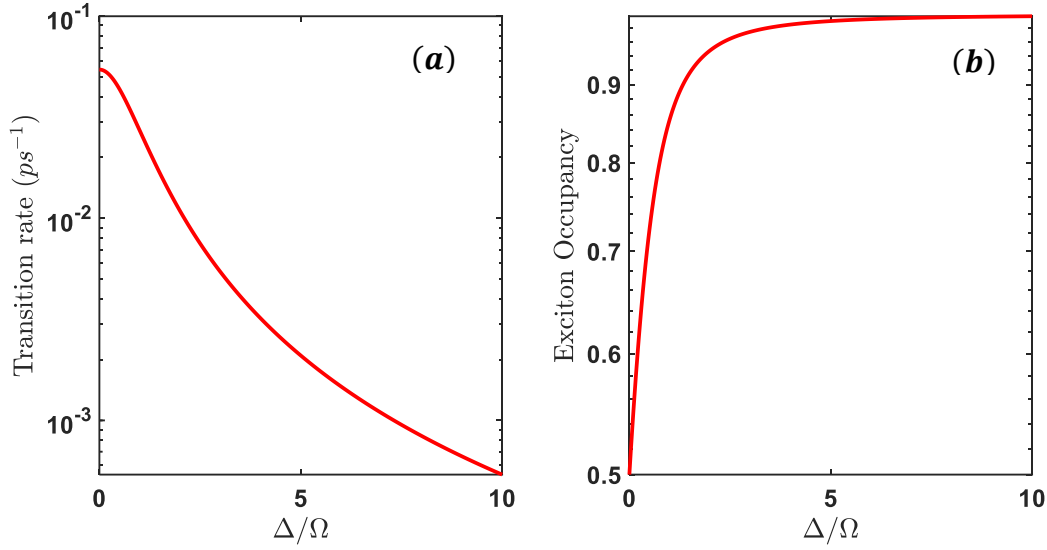


Fig. 8.4(a) Confined LO Phonon ($n = 1$) mode assisted transition rate between the dressed state for GaAs QD of radius 3nm at $T = 1K$. **(b)** Exciton occupancy (using Eq. (29)) in the final state at $T = 1K$.

We would like to point out that, because the phonon frequency $\omega_1 = \sqrt{\Delta^2 + \Omega^2}$, for any given detuning we can only have a specific value of Ω , hence we choose Δ/Ω to investigate all such possible combinations of allowed Δ and Ω affecting the transition rate.

It is clear from Fig. 8.4(a) that transition rate associated with confined LO phonon emission decreases (at all temperatures) with increase in Δ/Ω , however, from Fig. 8.4(b) it is observed that exciton occupancy increases with Δ/Ω , thus there exists a similar trade-off with confined LO modes as with bulk acoustic phonon modes [145]. At $T = 1K$, the maximum transition rate occurs at $\frac{\Delta}{\Omega} = 0$ which is of value $0.0545 ps^{-1}$ which corresponds to a relaxation time of $18.35 ps$ but the exciton occupancy is still 50%. We see that for exciton occupancy corresponding to 80% the corresponding relaxation time is $30.21 ps$. Also, we compare our results with transition rate triggered by acoustic phonon. As is well known, there exists very little mismatch between the acoustic properties of the QD material and the barrier material ($Al_xGa_{1-x}As$) in which the QD is

embedded so the acoustic confinement is negligible and the bulk acoustic phonon model can be used to evaluate the transition rates leading to the production of excitons. The bulk acoustic phonon density at low temperature is given as:

$$J_{acoustic}(\omega) = \frac{\omega^3}{4\pi^2 \hbar \rho_d c_{LA}^5} \left| \left(D^e e^{\frac{-\omega^2 a_e^2}{4c_{LA}^2}} - D^h e^{\frac{-\omega^2 a_h^2}{4c_{LA}^2}} \right) \right|^2 \quad (8.31)$$

where, $D^{e/h}$ is the electron/hole deformation potential, ρ_d is the material density, c_{LA} is the acoustic speed corresponding to longitudinal acoustic (LA) mode. We find that the acoustic spectral density peaks at $\omega = 16.46 \text{ cm}^{-1}$ with a peak value of 0.238 ps^{-1} . Using this value in Eq. (8.30) we find the maximum transition rate for acoustic phonon as a function of Δ/Ω in Fig. 8.5:

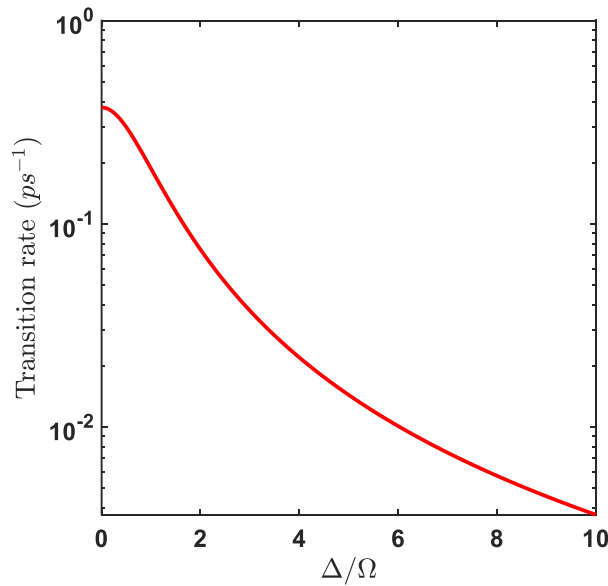


Fig. 8.5 Bulk acoustic phonon assisted transition rate in GaAs quantum dot of radius 3 nm at T = 1K.

Corresponding to exciton occupancy of 80%, the relaxation time for acoustic phonon at T = 1K is 4.39 ps hence it is 6.87 times (~ 7 times) less than the confined LO mode at the same temperature.

However, the average transition rate for confined LO mode for exciton occupancy above 80% for temperature $T \leq 10K$ is 0.0458 ps^{-1} (that corresponds to relaxation time of 22.38 ps) whereas for acoustic phonon mode, the average transition rate for $T \leq 10K$ is 0.3144 ps^{-1} (that corresponds to relaxation time of 3.26 ps). Hence, the exciton creation rate attributed to confined LO phonon is 6.87 times (~ 7 times) slower than acoustic phonon.

8.6 Conclusion

We investigated the role of confined LO phonons in GaAs QD taking a radius of 3 nm as representative of strong confinement limit. We find that phonon relaxation time corresponding to confined LO mode is approximately 7 times higher than acoustic phonon at low temperatures, $T \leq 10K$. It is clear that acoustic modes are the dominant phonon relaxation mechanism however at low temperatures ($\leq 10K$) the confined LO phonon cannot be neglected at all, hence it must be taken into account. Moreover, our results provide the theoretical basis for exciton preparation based of the use of optical-phonon-assisted processes rather than acoustic-phonon processes.

Chapter 9

Concluding Remarks

In this thesis theoretical framework necessary for modelling optical and acoustic phonons for studying their interaction with charge carriers in semiconductors and their nanostructures. We have studied wideband gap emerging semiconductors who are finding applications in high frequency and high power applications.

For Diamond, the hydrogenated surface (due to exposure to atmosphere) results in production of two dimensional hole gas. Since diamond is a non polar material, thus for proper accounting of phonon scattering we have quantized the Rayleigh wave, which are elliptically polarized surface waves localized on the surface, to properly model acoustic phonon in this structure. We have shown that surface acoustic phonon scattering limited mobility is about three times higher than the bulk acoustic modes. Also, we further examined a novel heterostructure consisting of two wide band gap semiconductors namely cubic boron nitride (cBN) and diamond. We have evaluated necessary conditions required to produce two dimensional electron gas at the interface, such structure is a well suited candidate for High Electron Mobility. We have shown that at room temperature the surface acoustic scattering is dominant as compared to the remote polar phonon leaking as evanescent mode in diamond from the cBN overlayer. The formalism developed in here can be applied to any such heterostructure which involves a polar and a non-polar material combination.

Further, we discussed the phonon decay rate in wurtzite crystals by taking 2H-SiC as an example, we took into account the directional variation in phonon velocity and their polarization into account. However, we find that the phonon lifetime is higher in the plane which contains the c-axis. This formalism can be used to find phonon decay rate in any wurtzite crystals. Of course, these calculation would encourage further experimental verification.

We did an in depth study to model phonon scattering in emerging wurtzite materials which depict strong electron – phonon coupling by applying the Thornber – Feynman path integral formalism duly considering the directional dependence of Fröhlich coupling. We demonstrated that the traditional phonon scattering modelled on the basis of Fermi’s golden rule (FGR) underestimates the energy loss by electron. This concept was further applied to cubic III – Nitrides and further extended to two dimensional Transition Metal Di-Chalcogenides. This work is very significant as it shows that we can find correction factors for FGR using the above approach, so we can still apply the FGR model and apply those correction factors to properly account for the strong coupling.

Lastly, we conclude that confined optical phonons can be deployed in qubit state preparation in quantum dot based qubit implementation, however acoustic phonons dominate the exciton generation but the role of confined LO phonons cannot be neglected and it must be taken into account while evaluating exciton generation rate. This work would definitely generate curiosity for further experimental validation.

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APPENDICES

Appendix A

Appendix A. I

$$F = \frac{b^3}{2} \int_l^L (y-l)^2 e^{-\alpha_{tl}y} e^{-b(y-l)} dy$$

$$F = \frac{b^3}{2} e^{-\alpha_{tl}l} \int_l^L (y-l)^2 e^{-(\alpha_{tl}+b)(y-l)} dy$$

Let, $\alpha_{tl} + b = m$ and $y - l = x$ and let $l_0 = L - l$

$$F = \frac{b^3}{2} e^{-\alpha_{tl}l} \int_0^{l_0} (x)^2 e^{-mx} dy$$

$$F = \frac{b^3}{2} \left[-\frac{l_0^2 e^{-ml_0}}{m} - \frac{2l_0 e^{-ml_0}}{m^2} - \frac{2(e^{-ml_0} - 1)}{m^3} \right]$$

Substituting for m and l_0 , we get:

$$F = \frac{b^3}{2} \left[-\frac{(L-l)^2 e^{-\alpha_{tl}L} e^{-bl_0}}{(\alpha_{tl} + b)} - \frac{2(L-l) e^{-\alpha_{tl}L} e^{-bl_0}}{(\alpha_{tl} + b)^2} - \frac{2 e^{-\alpha_{tl}l} (e^{-\alpha_{tl}L} e^{-bl_0} - 1)}{(\alpha_{tl} + b)^3} \right]$$

Appendix A (Continued)

Hence, Now squaring the above expression we get:

$$\begin{aligned}
 F^2 = & \frac{b^6}{4} \left[\frac{(L-l)^4 e^{-2\alpha_{tl}L} e^{-2b(L-l)}}{(\alpha_{tl} + b)^2} \right. \\
 & + \frac{4(L-l)^2 e^{-2\alpha_{tl}L} e^{-b(L-l)}}{(\alpha_{tl} + b)^4} \left(e^{-bl_0} + (e^{-\alpha_{tl}L} e^{-b(L-l)} - 1) \right) \\
 & + \frac{8(L-l) e^{-2\alpha_{tl}L} e^{-b(L-l)}}{(\alpha_{tl} + b)^5} (e^{-\alpha_{tl}L} e^{-b(L-l)} - 1) + \frac{4(L-l)^3 e^{-2\alpha_{tl}L} e^{-2b(L-l)}}{(\alpha_{tl} + b)^3} \\
 & \left. + \frac{4e^{-2\alpha_{tl}l}}{(\alpha_{tl} + b)^6} (e^{-\alpha_{tl}L} e^{-b(L-l)} - 1)^2 \right]
 \end{aligned}$$

Also,

$$\lim_{L \rightarrow \infty} (F)^2 = \frac{b^6}{4} \left(\frac{4e^{-2\alpha_{tl}l}}{(\alpha_{tl} + b)^6} \right) = \frac{b^6 e^{-2\alpha_{tl}l}}{(\alpha_{tl} + b)^6}$$

Appendix A (Continued)

Appendix A. II

$$A^2 = \frac{2 \alpha_{ts}^2 \alpha_{tl} / (\alpha_{tl} - \alpha_{ts})^2}{\beta_R^2 + \alpha_{ts}^2 \alpha_{tl} / (\alpha_{tl} - \alpha_{ts})}$$

Since, $\beta_R = q$

$$A^2 = \frac{2 \alpha_{ts}^2 \alpha_{tl} / (\alpha_{tl} - \alpha_{ts})^2}{q^2 + \alpha_{ts}^2 \alpha_{tl} / (\alpha_{tl} - \alpha_{ts})}$$

Moreover, α_{tl} and α_{ts} are not constants they are dependent on β_R as follows:

$$\alpha_{ts}^2 = \beta_R^2 - \left(\frac{\omega}{V_s}\right)^2$$

And,

$$\alpha_{tl}^2 = \beta_R^2 - \left(\frac{\omega}{V_l}\right)^2$$

But, we already know the relation between V_R and V_s as follows:

Hence, to simplify the expressions of F and A we can express α_{tl} and α_{ts} as below:

$$\alpha_{ts}^2 = \beta_R^2 - \left(\frac{\omega}{V_s}\right)^2$$

$$\alpha_{ts}^2 = \left(1 - \left(\frac{V_R}{V_s}\right)^2\right) \beta_R^2$$

$$\alpha_{ts} = \beta_R \sqrt{\left(1 - \left(\frac{V_R}{V_s}\right)^2\right)}$$

Appendix A (Continued)

So, let

$$\alpha_{ts} = s\beta_R = sq$$

and,

$$\alpha_{tl} = n\beta_R = nq$$

where, $s = \sqrt{\left(1 - \left(\frac{V_R}{V_s}\right)^2}\right)$ and $n = \sqrt{\left(1 - \left(\frac{V_R}{V_l}\right)^2}\right)$

Now, A can be simplified as follows:

$$A^2 = \frac{2 \alpha_{ts}^2 \alpha_{tl} / (\alpha_{tl} - \alpha_{ts})^2}{q^2 + \alpha_{ts}^2 \alpha_{tl} / (\alpha_{tl} - \alpha_{ts})}$$

$$A^2 = \frac{2 s^2 n / (n - s)^2}{q(1 + s^2 n / (n - s))} = \frac{A_2}{q}$$

Appendix B

$$\frac{1}{\tau^e} = \alpha \omega_{LO} \frac{1}{k} \sqrt{\frac{2m^* \omega_{LO}}{\hbar}} (N_q + 1) \ln \left[\frac{k + \sqrt{k^2 - \frac{2m^* \omega_{LO}}{\hbar}}}{k - \sqrt{k^2 - \frac{2m^* \omega_{LO}}{\hbar}}} \right]$$

Multiplying and dividing by $k + \sqrt{k^2 - \frac{2m^* \omega_{LO}}{\hbar}}$ inside the parenthesis, we get:

$$\frac{1}{\tau^e} = 2\alpha \omega_{LO} \frac{1}{k} \sqrt{\frac{2m^* \omega_{LO}}{\hbar}} (N_q + 1) \ln \left[\frac{\left(k + \sqrt{k^2 - \frac{2m^* \omega_{LO}}{\hbar}} \right)}{\sqrt{\frac{2m^* \omega_{LO}}{\hbar}}} \right]$$

$$\frac{1}{\tau^e} = 2\alpha \omega_{LO} \frac{1}{k} \sqrt{\frac{2m^* \omega_{LO}}{\hbar}} (N_q + 1) \ln \left[\sqrt{\frac{\hbar^2 k^2}{2m^* \hbar \omega_{LO}}} + \sqrt{\frac{\hbar^2 k^2}{2m^* \hbar \omega_{LO}} - 1} \right]$$

Now, substituting for α from Eq (1) and Electron energy $E_{el} = \frac{\hbar^2 k^2}{2m^*}$, we get:

$$\frac{1}{\tau^e} = \sqrt{\frac{2m^*}{E_{el}}} \frac{e^2 \omega_{LO} (N_q + 1)}{\hbar} \left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0} \right) \ln \left[\sqrt{\frac{E_{el}}{\hbar \omega_{LO}}} - 1 + \sqrt{\frac{E_{el}}{\hbar \omega_{LO}}} \right]$$

Appendix C

Appendix C. I

Herein, we analyze and evaluate $\bar{K}_{\beta'}(\xi)$ by expanding it to the second power in ξ .

Beginning with the discussion following Eq. 5 and using, $\cos(x) \approx 1 - \frac{x^2}{2}$ we obtain the following sequence of simplifications:

$$\bar{K}_{\beta'}(\xi) = \frac{1}{2} \frac{w_0^2}{v_0^2} \left[\left(\frac{v_0^2 - w_0^2}{w_0^2 v_0} \right) \times \left(\frac{\cosh\left(\frac{1}{2}\beta v_0\right) - 1 + \frac{v_0^2 \xi^2}{2}}{\sinh\left(\frac{1}{2}\beta v_0\right)} \right) + \frac{\xi^2}{\beta} + \frac{\beta}{4} \right]$$

$$\bar{K}_{\beta'}(\xi) = \frac{1}{2} \frac{w_0^2}{v_0^2} \left[\left(\frac{v_0^2 - w_0^2}{w_0^2 v_0} \right) \times \left(\frac{2\sinh^2\left(\frac{1}{4}\beta v_0\right)}{2\sinh\left(\frac{1}{4}\beta v_0\right)\cosh\left(\frac{1}{4}\beta v_0\right)} + \frac{(v_0^2 \xi^2/2)}{\sinh\left(\frac{1}{2}\beta v_0\right)} \right) + \frac{\xi^2}{\beta} + \frac{\beta}{4} \right]$$

$$\bar{K}_{\beta'}(\xi) = \frac{1}{2} \frac{w_0^2}{v_0^2} \left[\left(\frac{v_0^2 - w_0^2}{w_0^2 v_0} \right) \times \left(\tanh\left(\frac{1}{4}\beta v_0\right) + \frac{v_0^2 \xi^2/2}{\sinh\left(\frac{1}{2}\beta v_0\right)} \right) + \frac{\xi^2}{\beta} + \frac{\beta}{4} \right]$$

$$\bar{K}_{\beta'}(\xi) = \frac{1}{2\beta} \frac{\beta w_0^2}{v_0^2} \left[\left(\frac{v_0^2 - w_0^2}{w_0^2 v_0} \right) \times \tanh\left(\frac{1}{4}\beta v_0\right) + \frac{\beta}{4} \right] + \frac{\xi^2}{2\beta} \frac{w_0^2}{v_0^2} \left[\left(\frac{v_0^2 - w_0^2}{w_0^2 v_0} \right) \times \frac{v_0^2 \beta}{2\sinh\left(\frac{1}{2}\beta v_0\right)} + 1 \right]$$

$$\text{Letting } B_0 = \frac{\beta w_0^2}{v_0^2} \left[\left(\frac{v_0^2 - w_0^2}{w_0^2 v_0} \right) \times \tanh\left(\frac{1}{4}\beta v_0\right) + \frac{\beta}{4} \right]$$

we obtain,

$$\bar{K}_{\beta'}(\xi) = \frac{B_0}{2\beta} + \frac{\xi^2}{2\beta} \left[\frac{w_0^2}{v_0^2} \left(\frac{v_0^2 - w_0^2}{w_0^2 v_0} \right) \times \frac{v_0^2 \beta}{2\sinh\left(\frac{1}{2}\beta v_0\right)} + \frac{w_0^2}{v_0^2} \right]$$

Appendix C (Continued)

Now, writing $\frac{w_0^2}{v_0^2} = -\left(\frac{v_0^2 - w_0^2}{v_0^2}\right) + 1$

we find,

$$\bar{K}_{\beta'}(\xi) = \frac{B_0}{2\beta} + \frac{\xi^2}{2\beta} \left[\left(\frac{v_0^2 - w_0^2}{v_0^2} \right) \times \frac{\beta}{2\sinh\left(\frac{1}{2}\beta v_0\right)} - \left(\frac{v_0^2 - w_0^2}{v_0^2} \right) + 1 \right]$$

or,

$$\bar{K}_{\beta'}(\xi) = \frac{B_0}{2\beta} + \frac{\xi^2}{2\beta} \left[\left(\frac{v_0^2 - w_0^2}{v_0^2} \right) \times \left\{ \frac{v_0\beta}{2\sinh\left(\frac{1}{2}\beta v_0\right)} - 1 \right\} + 1 \right]$$

$$\text{Letting } A_0 = \left[\left(\frac{v_0^2 - w_0^2}{v_0^2} \right) \times \left\{ \frac{v_0\beta}{2\sinh\left(\frac{1}{2}\beta v_0\right)} - 1 \right\} + 1 \right]$$

We finally obtain,

$$\bar{K}_{\beta'}(\xi) = \frac{B_0}{2\beta} + \frac{A_0 \xi^2}{2\beta}$$

Appendix C (Continued)

Appendix C. II

To obtain Eq. 7.8, we begin with Eq. 7.6,

$$E = \int_{-\infty}^{\infty} d\xi \sum_q |C_q|^2 q \frac{\cos(\omega_q \xi)}{\sinh\left(\frac{1}{2}\beta\omega_q\right)} e^{-iq \cdot v(\xi+i\beta/2)} e^{-q^2 \bar{K}_{\beta'}(\xi)}$$

It is assumed that the applied electric field is in x-direction:

$$E = \int_{-\infty}^{\infty} d\xi \sum_q |C_q|^2 q_x \frac{\cos(\omega_q \xi)}{\sinh\left(\frac{1}{2}\beta\omega_q\right)} e^{-iq_x v(\xi+i\beta/2)} e^{-q^2 \bar{K}_{\beta'}(\xi)}$$

Taking the real part of above equation and substituting $\omega_q = 1$ (since phonons are assumed to be dispersion less and we work in Feynman units $\hbar = m_b = \omega_{Lo} = 1$) and $q_x = q \cos(\phi)$

$$\sum_q |C_q|^2 \rightarrow \frac{1}{(2\pi)^2} \int d^2 q |C_q|^2 = \frac{1}{(2\pi)^2} \int \sqrt{2\pi} \frac{\alpha}{q} q d\phi dq = \frac{\alpha}{2^{3/2}\pi} \int d\phi dq$$

Substituting, $\bar{K}_{\beta'}(\xi) = \frac{B_0}{2\beta} + \frac{A_0 \xi^2}{2\beta}$ and integrating w.r.t ξ first:

$$E = \frac{\alpha}{2^{3/2}\pi \sinh\left(\frac{1}{2}\beta\right)} \iint d\phi dq q \cos(\phi) e^{qv \cos(\phi)\beta/2} e^{\frac{-q^2 B_0}{2\beta}} \times \int_{-\infty}^{\infty} d\xi \left(\cos(\xi) \cos(qv \cos(\phi)\xi) e^{-q^2 \frac{A_0 \xi^2}{2\beta}} \right)$$

Appendix C (Continued)

Simplifying above expression with the terms involving ξ :

Let, $y \equiv \cos \phi$

$$\begin{aligned} & \cos(\xi) \cos(qvy\xi) e^{-q^2 \frac{A\xi^2}{2\beta}} \\ &= \int_{-\infty}^{\infty} d\xi \frac{1}{2} [\cos\{\xi(qvy+1)\}] e^{-q^2 \frac{A\xi^2}{2\beta}} + \int_{-\infty}^{\infty} d\xi \frac{1}{2} [\cos\{\xi(qvy-1)\}] e^{-q^2 \frac{A\xi^2}{2\beta}} \end{aligned}$$

Since,

$$\int_{-\infty}^{\infty} e^{-x^2 a} \cos(xb) = \frac{\sqrt{\pi}}{\sqrt{a}} e^{-b^2/4a}$$

So, after integrating over ξ we get:

$$\begin{aligned} E &= \frac{\alpha}{4\sqrt{\pi} \sinh\left(\frac{1}{2}\beta\right)} \cdot \sqrt{\frac{\beta}{A_0}} \\ &\times \iint d\phi dk \frac{q}{|q|} \cos(\phi) e^{qvy\beta/2} e^{\frac{-q^2 B_0}{2\beta}} \left(e^{\frac{-(\beta/2)(qvy+1)^2}{q^2 A_0}} + e^{\frac{-(\beta/2)(qvy-1)^2}{q^2 A_0}} \right) \end{aligned}$$

Simplifying the exponent of $e^{qvy\beta/2} e^{\frac{-(\beta/2)(qvy+1)^2}{q^2 A_0}}$, we get: $= \frac{-\beta}{2} \left[\left(\frac{yv}{\sqrt{A_0}} - \frac{q}{2} + \frac{1}{q} \right)^2 - \frac{q^2}{4} + 1 \right]$

Similarly, the exponent of $e^{qvy\beta/2} e^{\frac{-(\beta/2)(qvy-1)^2}{q^2 A_0}}$, we get: $= \frac{-\beta}{2} \left[\left(\frac{yv}{\sqrt{A_0}} - \frac{q}{2} - \frac{1}{q} \right)^2 - \frac{q^2}{4} - 1 \right]$

We have used $q\sqrt{A_0} \equiv q$, so that $\int dq \rightarrow \frac{1}{\sqrt{A_0}} \int dq$

Appendix C (Continued)

Using the above simplifications in the expression of E and substituting back $y \equiv \cos \phi$ with further algebraic simplifications we get:

$$E = \frac{\alpha}{4 \sinh\left(\frac{1}{2}\beta\right)} \cdot \sqrt{\frac{\beta}{\pi}} \cdot \frac{1}{A_0} \int_0^{2\pi} d\phi \cos(\phi) \int_0^\infty dk \frac{q}{|q|} \exp\left(-\frac{\beta k^2}{8A} \left[\frac{4B_0}{\beta^2} - A_0\right]\right) \\ \times \left(e^{\frac{-\beta}{2}} \exp\left(\frac{-\beta}{2} \left(\frac{\cos(\phi)v}{\sqrt{A}} - \frac{q}{2} + \frac{1}{q}\right)^2\right) + e^{\frac{\beta}{2}} \exp\left(\frac{-\beta}{2} \left(\frac{\cos(\phi)v}{\sqrt{A}} - \frac{q}{2} - \frac{1}{q}\right)^2\right) \right)$$

which is the form used in the analysis.

Appendix D

MATLAB codes used for calculations in chapter 2 and 3

Surface acoustic phonon scattering rate

```

clear
clc
%=====

hbar0 = 1.05457180e-34; % [J-s]
h0=2*pi*hbar0;          % Planck's constant
q0 = 1.60217662e-19;     % [Coulombs]
m0 = 9.10938356e-31;     % [kg]
kB = 1.38064852e-23;     % [J/K]
T = 200:50:450;
%T = 300;
kBT = kB*T;             % [J]
eps0 = 8.854187817e-12;  % [F/m]
c0 = 299792458;          % [m/s]
m_eff = 0.57;            % DOS effective mass
%m_eff = 0.444;          % conductivity effective mass
m = m_eff*m0;
wLO=1.1;                 % LO phonon frequency in cm-1
%w=2*pi*wLO*100*c0;      % Phonon frequency in s-1
Vl=18210;                 % [m/sec]
Vs=12300;                 % [m/sec]
epsr=5.7;                 % dielectric constant of damond
%Cd=5.5*q0;
Cd=8.7*q0;                % Deformation potential [J]
rho=3515;                 % density

s=0.2;

l=0e-9;
depth=l/1e-09;

Nh1 = 1e15;

%Ratio=(0.87+1.12*s)/(1+s);
b1=@(Nh) nthroot(((33*m*q0^2*Nh)/(8*eps0*epsr*hbar0^2)),3);
%b=arrayfun(b1,Nh);% old
b = b1(Nh1)
Vr=0.9117*Vs;

mu=sqrt(1-(Vr/Vs)^2);
nu=sqrt(1-(Vr/Vl)^2);

```

Appendix D (Continued)

```

A=(2*mu^2*nu/(nu-mu)^2)/(1+(2*mu^2*nu/(nu-mu)));

Eth = 1e3*m*(Vr^2)/(2*q0);

Elow = (0:0.01:Eth);
Eup= (Eth:0.01:300);

Ex= [Elow Eup];

for i = 1:length(T)
    C = b.^6*m*Cd^2*Vr^3/(pi*hbar0^2*rho*Vl^4);
    XE2=@(E) (A*C./(sqrt(2*m*E*1e-
3*q0/hbar0^2))).*integral(@(qe) ((exp(-
2*nu*qe*1).*(qe.^2).*(1+1./(exp(hbar0*Vr*qe./(kB*T(i)))-
1)))./((nu*qe+b).^6)) ...
    .*((1./(sqrt(abs(1-(hbar0^2./(2*m*(E*1e-
3*q0))))).*(qe./2+m*Vr./hbar0).^2))),0,(2*sqrt(2*m*E*1e-3*q0) -
2*m*Vr)/hbar0,'ArrayValued',true );

    XE2R=arrayfun(XE2,Eup);

    XA1=@(E) (A*C./(sqrt(2*m*E*1e-
3*q0/hbar0^2))).*integral(@(qe) ((exp(-
2*nu*qe*1).*(qe.^2).*(1./(exp(hbar0*Vr*qe./(kB*T(i)))-
1)))./((nu*qe+b).^6)) ...
    .*((1./(sqrt(abs(1-(hbar0^2./(2*m*(E*1e-3*q0))))).*(qe./2-
m*Vr./hbar0).^2))),(-2*sqrt(2*m*E*1e-3*q0) +
2*m*Vr)/hbar0,(2*sqrt(2*m*E*1e-3*q0) +
2*m*Vr)/hbar0,'ArrayValued',true );

    XA2=@(E) (A*C./(sqrt(2*m*E*1e-
3*q0/hbar0^2))).*integral(@(qe) ((exp(-
2*nu*qe*1).*(qe.^2).*(1./(exp(hbar0*Vr*qe./(kB*T(i)))-
1)))./((nu*qe+b).^6)) ...
    .*((1./(sqrt(abs(1-(hbar0^2./(2*m*(E*1e-3*q0))))).*(qe./2-
m*Vr./hbar0).^2))),0,(2*sqrt(2*m*E*1e-3*q0) +
2*m*Vr)/hbar0,'ArrayValued',true );

    XA1R=arrayfun(XA1,Elow); % absorption rate array until Eth
    XA2R=arrayfun(XA2,Eup); % absorption rate array after Eth
    XAR=[XA1R XA2R]; % Full absorption rate array

```

Appendix D (Continued)

```

TE1R = zeros(1,length(XA1R)); % Emission rate is zero until
the threshold energy, length is equal to absorption array
TE2R = XE2R;
TER = [TE1R TE2R];
iTAU = TER + XAR;
TAU = 1./iTAU;
idx = find(isnan(TAU));
TAU(idx)=[];

% -----%
This snippet computes mobility by doing energy average integral
%

Xtot1 = @(E)1./(XA1(E));
Xtot2 = @(E)1./(XE2(E)+XA2(E));

XEN1=integral(@(E)((E*1e-3*q0)).*exp(-((E*1e-
3*q0))/(kB*T(i))).*(Xtot1(E)),0,Eth,'ArrayValued',true);
XEN2=integral(@(E)((E*1e-3*q0)).*exp(-((E*1e-
3*q0))/(kB*T(i))).*(Xtot2(E)),Eth,inf,'ArrayValued',true);

XEN= XEN1+XEN2;
XED=integral(@(E)((E*1e-3*q0)).*exp(-((E*1e-
3*q0))/(kB*T(i))),0,inf,'ArrayValued',true);

Mobility_continuous(i)=(q0/(m)).*(XEN/XED)*1e4
%

end

%
semilogy(T,Mobility_continuous,'LineWidth',4.0)
hold on
set(gca,'FontSize',24,'FontWeight','bold')
grid minor

```

Appendix E

This program computes the scattering due to remote polar phonons leaking as evanescent mode from cBN over layer in chapter 3

```
% REMOTE POLAR PHONON SCATTERING in c-BN/DIAMOND
hbar0=1.0545887e-27;    % [erg-s]
c0=2.99792458e10;     % [cm/s]
fx=6.242e11;          % conversion factor [erg] to [eV]
q0=4.80320420e-10;    % elementary charge [ESU]

m0 = 9.10938356e-28;   % [gram]
kB = 1.38064852e-16;   % [erg/K]
T = 300;              % [K]
kBT = kB*T;           % [erg]

pic2 = 2*pi*c0;
m_eff=0.57;% Effective Mass of Electron in Diamond
m=m_eff*m0;
epsr=5.7; % Dielectric Constant Diamond
wLO = 1285*pic2;
wTO = 1040*pic2;
einf = 4.54; % c-BN dielectric Constant at w = infinity
Nh = 1e12; % Sheet Density
B = (48*pi*m*q0^2*Nh)/(epsr*hbar0^2);
b = nthroot(B,3);
d = 1e-7;

wS =
@(q) sqrt((wTO^2+einf*wLO^2*tanh(0.5*d*q))/(1+einf*tanh(0.5*d*q)));
wA =
@(q) sqrt((wTO^2+einf*wLO^2*coth(0.5*d*q))/(1+einf*coth(0.5*d*q)));

%E = (0:0.001:0.5)/fx;
E = linspace(0,0.5,500)/fx;
k = sqrt(2*m*E/hbar0^2);
%
%-----
% Emission Symmetric 0 <phi<pi
%-----
for i =1:length(E)
    [Q1,Q2,Q3,Q4,Q5,Q6,Q7,Q8] = QlimE(k(i),d);
    if Q1==0 && Q2 ==0
        Emission1S(i) = 0;
```

Appendix E (Continued)

```

else
    F1 = @(q) sqrt(abs(1-
    ((m*wS(q)/(hbar0*k(i)*q))+q/(2*k(i))).^2));
    NqS = @(q) 1./ (exp(hbar0*wS(q)./kBT)-1);
    D1DwS = @(q) (einf)*(2*wS(q)*(wLO^2-wTO^2)./((wS(q)).^2-
wTO^2).^2); % derivative of dielectric function
    DenS = @(q) D1DwS(q)*tanh(0.5*d*q);
    %X = @(q) (b./(b+q).^6);
    C = (2*m*q0^2)/(hbar0^2*epsr^2);
    D = @(q) (b./(b+q)).^6*(1/DenS(q))*(NqS(q)+1);
    I1S = @(q) C*(D(q)/q)*(1/F1(q))*(1/k(i));
    E1 = integral(@(q) I1S(q), Q1, Q2, 'ArrayValued', true);

    Emission1S(i) = E1;
end

end

%-----
% Emission Symmetric pi < phi < 2*pi
%-----
for i =1:length(E)
    [Q1,Q2,Q3,Q4,Q5,Q6,Q7,Q8] = QlimE(k(i),d);
    if Q3==0 && Q4 ==0
        Emission2S(i) = 0;
    else
        F1 = @(q) sqrt(abs(1-
        ((m*wS(q)/(hbar0*k(i)*q))+q/(2*k(i))).^2));
        NqS = @(q) 1./ (exp(hbar0*wS(q)./kBT)-1);
        D1DwS = @(q) (einf)*(2*wS(q)*(wLO^2-wTO^2)./((wS(q)).^2-
wTO^2).^2); % derivative of dielectric function
        DenS = @(q) D1DwS(q)*tanh(0.5*d*q);
        %X = @(q) (b./(b+q).^6);
        C = (2*m*q0^2)/(hbar0^2*epsr^2);
        D = @(q) (b./(b+q)).^6*(1/DenS(q))*(NqS(q)+1);
        I2S = @(q) C*(D(q)/q)*(1/F1(q))*(1/k(i));
        E2 = integral(@(q) I2S(q), Q3, Q4, 'ArrayValued', true);

        Emission2S(i) = E2;
    end
end

end

```

Appendix E (Continued)

```

EmissionS = Emission1S + Emission2S;

%
%-----
% Emission Anti - Symmetric Mode 0 < phi < pi
% -----
for i =1:length(E)
    [Q1,Q2,Q3,Q4,Q5,Q6,Q7,Q8] = QlimE(k(i),d);
    if Q5==0 && Q6 ==0
        Emission1A(i) = 0;
    else
        F1A = @(q) sqrt(abs(1-
        ((m*WA(q)/(hbar0*k(i)*q))+q/(2*k(i))).^2));
        NqA = @(q) 1./(exp(hbar0*WA(q)./kBT)-1);
        D1DwA = @(q) (einf)*(2*WA(q)*(wLO^2-wTO^2)./((WA(q)).^2-
wTO^2).^2); % derivative of dielectric function
        DenA = @(q) D1DwA(q)*tanh(0.5*d*q);
        %X = @(q) (b./(b+q).^6);
        C = (2*m*q0^2)/(hbar0^2*epsr^2);
        D = @(q) (b./(b+q)).^6*(1/DenA(q))*(NqA(q)+1);
        I1A = @(q) C*(D(q)/q)*(1/F1A(q))*(1/k(i));
        E1A = integral(@(q) I1A(q),Q5,Q6,'ArrayValued',true);

        Emission1A(i) = E1A;
    end
end

%
%-----
% Emission Anti-Symmetric pi < phi < 2*pi
% -----
for i =1:length(E)
    [Q1,Q2,Q3,Q4,Q5,Q6,Q7,Q8] = QlimE(k(i),d);
    if Q7==0 && Q8 ==0
        Emission2A(i) = 0;
    else
        F1 = @(q) sqrt(abs(1-
        ((m*WA(q)/(hbar0*k(i)*q))+q/(2*k(i))).^2));
        NqA = @(q) 1./(exp(hbar0*WA(q)./kBT)-1);
        D1DwA = @(q) (einf)*(2*WA(q)*(wLO^2-wTO^2)./((WA(q)).^2-
wTO^2).^2); % derivative of dielectric function

```

Appendix E (Continued)

```

DenA = @(q) D1DwA(q)*tanh(0.5*d*q);
%X = @(q) (b./(b+q).^6);
C = (2*m*q0^2)/(hbar0^2*epsr^2);
D = @(q) (b./(b+q)).^6*(1/DenA(q))*(NqA(q)+1);
I2A = @(q) C*(D(q)/q)*(1/F1(q))*(1/k(i));
E2A = integral(@(q) I2A(q),Q7,Q8,'ArrayValued',true);
Emission2A(i) = E2A;
end

end

set(gca,'FontSize',24,'FontWeight','bold')
EmissionA = Emission1A + Emission2A;
EmissionT = EmissionA +EmissionS;
%
figure(5)
semilogy(E*fx,EmissionS,'k','LineWidth',3)
hold on
semilogy(E*fx,EmissionA,'r','LineWidth',3)
grid minor
set(gca,'FontSize',24,'FontWeight','bold')
ylabel('1/\tau ','FontSize',22,'FontWeight','bold')
xlabel('Energy (eV)','FontSize',22,'FontWeight','bold')
legend('Symmetric Mode','Anti-Symmetric Mode')
title('Emssion Rates ')
hold on
xlim([0 0.5])
%}
%
figure(6)
semilogy(E*fx,EmissionT,'LineWidth',3)
grid minor
set(gca,'FontSize',24,'FontWeight','bold')
ylabel('1/\tau ','FontSize',22,'FontWeight','bold')
xlabel('Energy (eV)','FontSize',22,'FontWeight','bold')
title('Total Emssion Rate ')

```

Appendix E (Continued)

```

%-----
% Absorption Symmetric 0 < phi < pi
% -----

for i =1:length(k)
    [Q1,Q2,Q3,Q4,Q5,Q6,Q7,Q8] = limSymA(k(i),d);
    qminAbS = Q1;
    qmaxAbS = Q2;

    F1 = @(q) sqrt(abs(1-(q/(2*k(i)) -
(m*wS(q)/(hbar0*k(i)*q)).^2)));
    NqS = @(q) 1./(exp(hbar0*wS(q)./kBT)-1);
    D1DwS = @(q) (einf)*(2*wS(q)*(wLO^2-wTO^2)./(wS(q)).^2-
wTO^2).^2); % derivative of dielectric function
    DenS = @(q) D1DwS(q)*tanh(0.5*d*q);
    %X = @(q) (b./(b+q).^6);
    C = (2*m*q0^2)/(hbar0^2*epsr^2);
    D = @(q) (b./(b+q)).^6*(1/DenS(q))*(NqS(q));
    I1S = @(q) C*(D(q)/q)*(1/F1(q))*(1/k(i));
    A1S = 2*integral(@(q) I1S(q),Q1,Q2,'ArrayValued',true);
    Absorption1S(i) = A1S;
end

%}

%
%-----
% Absorption Symmetric pi < phi < 2*pi
% -----

%
for i =1:length(E)
    [Q1,Q2,Q3,Q4,Q5,Q6,Q7,Q8] = limSymA(k(i),d);

    F1 = @(q) sqrt(abs(1-(q/(2*k(i)) -
(m*wS(q)/(hbar0*k(i)*q)).^2)));
    NqS = @(q) 1./(exp(hbar0*wS(q)./kBT)-1);
    D1DwS = @(q) (einf)*(2*wS(q)*(wLO^2-wTO^2)./(wS(q)).^2-
wTO^2).^2); % derivative of dielectric function
    DenS = @(q) D1DwS(q)*tanh(0.5*d*q);
    %X = @(q) (b./(b+q).^6);
    C = (2*m*q0^2)/(hbar0^2*epsr^2);
    D = @(q) (b./(b+q)).^6*(1/DenS(q))*(NqS(q));

```

Appendix E (Continued)

```

I1S = @(q)C*(D(q)/q)*(1/F1(q))*(1/k(i));
A2S = 2*integral(@(q)I1S(q),Q3,Q4,'ArrayValued',true);
Absorption2S(i) = A2S;
end

AbsorptionS = Absorption1S +Absorption2S;
%-----
% Absorption Anti-Symmetric 0 < phi < pi
% -----

for i =1:length(E)
    [Q1,Q2,Q3,Q4,Q5,Q6,Q7,Q8] = limSymA(k(i),d);

    F1 = @(q)sqrt(abs(1-(q/(2*k(i))-(
(m*wA(q)/(hbar0*k(i)*q)).^2)));
    NqA = @(q)1./(exp(hbar0*wA(q)./kBT)-1);
    D1DwA = @(q)(einf)*(2*wA(q)*(wLO^2-wTO^2)./(wA(q)).^2-
wTO^2).^2); % derivative of dielectric function
    DenA = @(q)D1DwA(q)*tanh(0.5*d*q);
    %X = @(q)(b./(b+q).^6);
    C = (2*m*q0^2)/(hbar0^2*epsr^2);
    D = @(q)(b./(b+q)).^6*(1/DenA(q))*(NqA(q));
    I1A = @(q)C*(D(q)/q)*(1/F1(q))*(1/k(i));
    A1A = 2*integral(@(q)I1A(q),Q5,Q6,'ArrayValued',true);
    Absorption1A(i) = A1A;
end
%-----
% Absorption Anti-Symmetric pi < phi < 2*pi
% -----

for i =1:length(E)
    [Q1,Q2,Q3,Q4,Q5,Q6,Q7,Q8] = limSymA(k(i),d);

    F1 = @(q)sqrt(abs(1-(q/(2*k(i))-(
(m*wA(q)/(hbar0*k(i)*q)).^2)));
    NqA = @(q)1./(exp(hbar0*wA(q)./kBT)-1);
    D1DwA = @(q)(einf)*(2*wA(q)*(wLO^2-wTO^2)./(wA(q)).^2-
wTO^2).^2); % derivative of dielectric function
    DenA = @(q)D1DwA(q)*tanh(0.5*d*q);
    %X = @(q)(b./(b+q).^6);
    C = (2*m*q0^2)/(hbar0^2*epsr^2);
    D = @(q)(b./(b+q)).^6*(1/DenA(q))*(NqA(q));
    I1A = @(q)C*(D(q)/q)*(1/F1(q))*(1/k(i));
    A2A = 2*integral(@(q)I1A(q),Q7,Q8,'ArrayValued',true);
    Absorption2A(i) = A2A;
end

```

Appendix E (Continued)

```

AbsorptionA = Absorption1A+Absorption2A;

AbsorptionT = AbsorptionS+AbsorptionA;
%
figure(7)
semilogy(E*fx,AbsorptionS,'k','LineWidth',3)
hold on
semilogy(E*fx,AbsorptionA,'r','LineWidth',3)
set(gca,'FontSize',24,'FontWeight','bold')
ylabel('1/\tau ','FontSize',22,'FontWeight','bold')
xlabel('Energy (eV)','FontSize',22,'FontWeight','bold')
legend('Symmetric Mode','Anti-Symmetric Mode')
title('Absorption Rates')
grid minor
%ylim([1e11 1e13])
xlim([0 0.5])
%}
%
figure(8)
semilogy(E*fx,AbsorptionT,'LineWidth',3)
set(gca,'FontSize',24,'FontWeight','bold')
ylabel('1/\tau ','FontSize',22,'FontWeight','bold')
xlabel('Energy (eV)','FontSize',22,'FontWeight','bold')
title('Total Absorption Rate')
grid minor
%}
%
figure(9)
semilogy(E*fx,AbsorptionT+EmissionT,'LineWidth',3)
set(gca,'FontSize',24,'FontWeight','bold')
ylabel('1/\tau (sec^-^1) ','FontSize',22,'FontWeight','bold')
xlabel('Energy (eV)','FontSize',22,'FontWeight','bold')
title('Total Scattering Rate')
grid minor
%}

%-----

```

Appendix F

MATLAB codes used for calculations in chapter 4

Computation of phonon decay rate in XY plane

```
hbar0 = 1.05457180e-34; % [J-s]
q0 = 1.60217662e-19; % [Coulombs]
f = (5:0.5:10)*1e12;
w=2*pi*f;
A1 = [0.0024 -0.0006 -0.0004 0 0 0];
A2 = [-0.0006 0.0024 -0.0004 0 0 0];
A3 = [-0.0004 -0.0004 0.0022 0 0 0];
A4 = [0 0 0 0.007 0 0];
A5 = [0 0 0 0 0.007 0];
A6 = [0 0 0 0 0 0.0061];
A = [A1;A2;A3;A4;A5;A6];
C = 1e9*inv(A);
rho=6.154e3; % density
C11= C(1,1);
C12= C(1,2);
C44 = C(4,4);
C33 = C(4,4);
C66 = C(6,6);
v1 =sqrt(C11/rho);
vt =sqrt(C66/rho);
vt1=vt;
vt2=sqrt((C44)/(2*rho));
d=1.75; % delta
d2 = v1/vt2;
d3 = vt1/vt2;
%v1=7.906e3; % longitudinal velocity
%vt=4.109e3; % transverse velocity
L=1.934e11; % lambda
m=1.434e11; % mu
b=-0.886e11; % beta
g=-0.1185e11; % little gamma
%x0=(d-1)/(d+1); % x0 lower limit of integration
C1 = (b+L+2*(g+m));
C2 = (b+2*g+m);
C3 = (b+L);
C4 = 2*(g+m);
x1a = (d-1)/2;
x2a=(d+1)/2;
Ca = (hbar0*w.^5)/(32*pi*rho^3*v1^6*vt^3);

fla = @(x) (2*x.^2-2*x*d+(d^2-1))^2;
```

Appendix F (Continued)

```

f2a = @(x) (d^2-1) * ((2*x-d).^2-1);

Fa = @(x) (1./ (16*x.^2.* (d-x).^2)) .* (C1*f1a(x)+C2*f2a(x)).^2;

gamma2a = Ca*integral(@(x) Fa(x), x1a, x2a, 'ArrayValued', true);

Cb = (hbar0*w.^5) / (32*pi*rho^3*v1^6*vt1*vt2^2);

f1b= @(x) ((1-x.^2)-(d2-d3*x).^2) ./ (2*x);
f2b=@(x) (0.5*((1-x.^2)+(d2-d3*x).^2))*((1+x.^2)-(d2-
d3*x).^2) ./ (2*x));

Fb = @(x) (x.^2./ (d2-d3*x).^2) * (C3*f1b(x)+C4*f2b(x)).^2;

a1 = ((1-d2*d3)-sqrt((1-d2*d3)^2-(1-d3^2)*(1-d2^2)))/(1-d3^2);
b1 = ((1-d2*d3)+sqrt((1-d2*d3)^2-(1-d3^2)*(1-d2^2)))/(1-d3^2);
b2 = (-(1+d2*d3)+sqrt((1+d2*d3)^2-(1-d3^2)*(1-d2^2)))/(1-d3^2);

gamma2b = Cb*integral(@(x) Fb(x), b2, 1, 'ArrayValued', true);

figure (1)
semilogy(f/1e12, gamma2a, 'k', 'LineWidth', 3)
hold on
semilogy(f/1e12, gamma2b, 'r', 'LineWidth', 3)
hold on
semilogy(f/1e12, gamma2b+gamma2a, 'g', 'LineWidth', 3)
set(gca, 'FontSize', 24, 'FontWeight', 'bold')
xlabel('THz', 'FontSize', 24, 'FontWeight', 'bold')
ylabel('\Gamma_2[s^{-1}]', 'FontSize', 24, 'FontWeight', 'bold')
legend('\Gamma_a_2', '\Gamma_b_2', '\Gamma_2')
title('\Gamma Process 2 in XY plane ',
'FontSize', 24, 'FontWeight', 'bold')
grid minor

Z= (2*b+4*g+L+3*m);

CP1= ((hbar0*w.^5) / (256*pi*rho^3)) * ((d^2-1)/v1^9)*Z^2;

FP1 = @(x) (0.5./x.^2) .* (1-x.^2).^2 .* ((1+x).^2-d^2*(1-
x).^2) .* ((1+x.^2)-d^2*(1-x).^2).^2;

```

Appendix F (Continued)

```
gamma1 = CP1*integral(@(x)FP1(x),(d-
1)/(d+1),1,'ArrayValued',true);

figure (2)
semilogy(f/1e12,gamma1,'k','LineWidth',3)

set(gca,'FontSize',24,'FontWeight','bold')
xlabel('THz','FontSize',24,'FontWeight','bold')
ylabel('\Gamma_1[s^{-1}]','FontSize',24,'FontWeight','bold')
title('\Gamma Process 1 XY plane ',
'FontSize',24,'FontWeight','bold')
grid minor

figure (3)
semilogy(f/1e12,gamma1,'k','LineWidth',3)
hold on
semilogy(f/1e12,gamma2b+gamma2a,'r','LineWidth',3)

set(gca,'FontSize',24,'FontWeight','bold')
xlabel('THz','FontSize',24,'FontWeight','bold')
ylabel('\Gamma[s^{-1}]','FontSize',24,'FontWeight','bold')
legend('\Gamma_1','\Gamma_2')
title('\Gamma Process 1 and 2 in XY plane ',
'FontSize',24,'FontWeight','bold')
grid minor
```

For the plane normal to XY plane
SiC_NormalThetaVx.m

```
% This program finds the root of Energy conervation equation
contained ...
% in the argument of dirac-delta function.
% This program is dedicated for plane NORMAL to XY plane

%close all; clear; clc;
A1 = [0.0024 -0.0006 -0.0004 0 0 0];
A2 = [-0.0006 0.0024 -0.0004 0 0 0];
A3 = [-0.0004 -0.0004 0.0022 0 0 0];
A4 = [0 0 0 0.007 0 0];
A5 = [0 0 0 0 0.007 0];
A6 = [0 0 0 0 0 0.0061];
A = [A1;A2;A3;A4;A5;A6];
C = 1e9*inv(A);
rho=3.21e3; % density
```

Appendix F (Continued)

```
% plane containing c-axis

% pure shear mode polarized normal to the plane
Stn = @(t) sqrt(rho./(C(6,6)*(sin(t)).^2+C(4,4)*(cos(t)).^2));
Vtn = @(t) 1./Stn(t);

% quasi shear wave in-plane

Y1 = @(t) ((C(1,1)-C(4,4))*(sin(t)).^2+(C(4,4)-C(3,3))*(cos(t)).^2).^2+((C(1,3)+C(4,4))*sin(2*t)).^2;
Xp = @(t) C(1,1)*(sin(t)).^2+C(3,3)*(cos(t)).^2+C(4,4)-sqrt(Y1(t));
Stp = @(t) sqrt(2*rho)./sqrt(Xp(t));
Vtp = @(t) 1./Stp(t);

% quasi longitudinal mode in-plane

Xn =
    @(t) C(1,1)*(sin(t)).^2+C(3,3)*(cos(t)).^2+C(4,4)+sqrt(Y1(t));
Slp = @(t) sqrt(2*rho)./sqrt(Xn(t));
Vlp = @(t) 1./Slp(t);

r = @(t) Vlp(t)./Vtp(t);
r1 = @(t) Vtn(t)./Vtp(t);

% Process-I x limit
x1 = 0.301:0.001:0.999;

% Process-II x limit
% (IIa and b have same x limit)
x2= 0.431:0.001:0.999;
n=1;
j=1;

% Process-I x vs theta calculation
% This loop computes the root of dirac delta argument
% T1 matrix stores x vs theta. y1 are the theta roots
for i =1:length(x1)
    f1 = @(t) r(t)-sqrt(1+x1(i)^2-2*x1(i).*cos(t))./(1-x1(i));

    y1 = fzero(f1,[0 pi]);
```

Appendix F (Continued)

```

T1(n,:) = [x1(i) y1];

n = n+1;

end
% Process-IIa&b x vs theta calculation
% This loop computes the root of dirac delta argument
% T2a matrix stores x vs theta for Process IIa.
% T2b matrix stores x vs theta for Process IIb.
% y2a and y2b are theta roots for IIa & b respectively
for i = 1:length(x2)

    f2a = @(t) r(t)-x2(i)-sqrt(1+x2(i)^2-2*x2(i).*cos(t));
    f2b = @(t) r(t)-x2(i)-r1(t).*sqrt(1+x2(i)^2-2*x2(i).*cos(t));

    y2a = fzero(f2a,[0 pi]);
    y2b = fzero(f2b,[0 pi]);

    T2a(j,:) = [x2(i) y2a];
    T2b(j,:) = [x2(i) y2b];
    j = j+1;

end

plot(T1(:,1), (180/pi)*T1(:,2), 'g', 'LineWidth', 3)
hold on
plot(T2a(:,1), (180/pi)*T2a(:,2), 'k', 'LineWidth', 3)
hold on
plot(T2b(:,1), (180/pi)*T2b(:,2), 'r', 'LineWidth', 3)

xlabel("x = q'/q")
ylabel('\theta [in deg]')
title ('Process I & II: Variation of \theta vs x in XZ plane')
legend('\Gamma_1', '\Gamma^a_2', '\Gamma^b_2')
xlim([0.2 1])
ylim([0 120])

set(gca, 'FontSize', 24, 'LineWidth', 3)

```

Appendix F (Continued)

```

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% This is Final code for Normal plane
% This code evaluates and plots phonon decay rate in 2H-SiC
% This code is for plane NORMAL to XY plane i.e plane containing
c-axis.

hbar0 = 1.05457180e-34; % [J-s]
q0 = 1.60217662e-19; % [Coulombs]
fr = (5:0.5:10)*1e12;
w=2*pi*fr;
rho=3.21e3; % density
L=1.934e11; % lambda
m=1.434e11; % mu
b=-0.886e11; % beta
g=-0.1185e11; % little gamma
Z = 2*b+4*g+L+3*m;
C1 = (b+L+2*(g+m));
C2 = (b+2*g+m);
C3 = (b+L);
C4 = 2*(g+m);
SiC_NormalThetaVx

t1 = T1(:,2)';
t2a = T2a(:,2)';
t2b = T2b(:,2)';
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% roots of dirac-delta function: cos(theta) = F(x)
Fun1 = cos(t1);
Fun2a = cos(t2a);
Fun2b = cos(t2b);

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%% Process-2%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% Derivatives of argument of dirac-delta function
%
%f1 = @(t)r(t)-sqrt(1+x1.^2-2*x1.*cos(t))./(1-x1);
f2a = @(t)r(t)-x2-sqrt(1+x2.^2-2*x2.*cos(t));
f2b = @(t)r(t)-x2-r1(t).*sqrt(1+x2.^2-2*x2.*cos(t));

% Velocity
V1 = Velocity(cos(t2a));
V2 = Velocity(cos(t2b));

```

Appendix F (Continued)

```
Vl_a = V1(1,:);
Vtp_a = V1(2,:);
Vl_b = V2(1,:);
Vtp_b = V2(2,:);
Vtn_b = V2(3,:);

% ratio of longitudinal to shear velocity
Rsa = Vl_a./Vtp_a;
Rsb = Vl_b./Vtp_b;
Rls = Vtn_b./Vtp_b;

% differentiation of ratios
Rdiff_a = dydx(Rsa,cos(t2a));
Rdiff_b = dydx(Rsb,cos(t2b));
Rldiff = dydx(Rls,cos(t2b));

%square root term in the diracdelta argument
ha = sqrt(1+x2.^2-2*x2.*cos(t2a));
hb = Rls.*sqrt(1+x2.^2-2*x2.*cos(t2b));

% derivative of square root term
Fa = Rdiff_a +x2./ha;
Fb = Rdiff_b +Rls.*x2./hb-Rldiff.*(hb./Rls);

% absolute value of derivative of argument of dirac-delta
function
F2a_der = abs(Fa);
F2b_der = abs(Fb);

Vl1a = Vl_a;
Vl1b = Vl_b;
Vt1a = Vtp_a;
Vt1b = Vtp_b;
Vt2b = Vtn_b;

G2a = (((x2.^3).*(C1*(x2-cos(t2a)).^2-C2*(1-
cos(t2a).^2)).^2))./((Vl1a.^6.*Vt1a.^3).*(1+x2.^2-
2*x2.*cos(t2a)).^(3/2)));
```

Appendix F (Continued)

```
% Integrand process 2b
G2b = ((x2.^3).* (C3*(cos(t2b)-x2) + C4*(1-
x2.*cos(t2b)).*cos(t2b)).^2)./(Vl1b.^6.*Vt1b.^2.*Vt2b.*sqrt(1+x2
.^2-2*x2.*cos(t2b)));

I2a = G2a./F2a_der;
I2b = G2b./F2b_der;

%
% Integrating
x22 =x2;
x22(19)=[];
I2a(19)=[];
rate2a = trapz(x22,I2a);
rate2b = trapz(x2,I2b);

rate_P2a = ((hbar0*w.^5)./(32*pi*rho^3)).*(rate2a);
rate_P2b = ((hbar0*w.^5)./(32*pi*rho^3)).*(rate2b);
rate_2 = rate_P2a+rate_P2b;
figure(3)
semilogy(fr/1e12, rate_P2a,'k','LineWidth',3)
hold on
semilogy(fr/1e12, rate_P2b,'r','LineWidth',3)
hold on
semilogy(fr/1e12, rate_2,'g','LineWidth',3)
grid minor
xlabel('f (THz)');
ylabel('\Gamma_a_2');
legend('\Gamma_a_2','\Gamma_b_2','\Gamma_2')
title('Process IIa: Plane normal to XY plane')
set(gca,'FontSize',24,'FontWeight','bold')

%}

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%% Process-1%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

% Velocity
VA = Velocity(cos(t1));
Vl = VA(1,:);
Vt = VA(2,:);
Rs = Vl./Vt;

Rsdiff = dydx(Rs,cos(t1));
```

Appendix F (Continued)

```

G1_N = ((x1.^3).*(1-x1.^2).^2).*sin(t1).^2.*cos(t1).^2;

G1_D = V1.^7.*Vt.^2.*((1+x1.^2)-2*x1.*cos(t1)).^(3/2);
G1 = G1_N./G1_D;

F1_der = Rsdiff.*(1-x1) + x1./sqrt((1+x1.^2)-2*x1.*cos(t1));
I1 = G1./abs(F1_der);
rate1 = trapz(x1,I1);

rate_P1 = ((hbar0*w.^5*Z.^2)./(32*pi*rho^3)).*(rate1);
figure(4)
semilogy(fr/1e12, rate_P1,'k','LineWidth',3)
hold on
semilogy(fr/1e12, rate_2,'r','LineWidth',3)
grid minor
xlabel('f (THz)');
ylabel('\Gamma_1 , \Gamma_2');
legend('\Gamma_1', '\Gamma_2')
title('Process I & II: Plane normal to XY plane')
set(gca,'FontSize',24,'FontWeight','bold')

% function Description
% INPUT: Cosine (t) array [from x vs cos(t) table]
% OUTPUT: XZ plane(plane containing c-axis) velocities

function velocity_matrix = Velocity(cost)

rho=6.154e3; % density
A1 = [0.0024 -0.0006 -0.0004 0 0 0];
A2 = [-0.0006 0.0024 -0.0004 0 0 0];
A3 = [-0.0004 -0.0004 0.0022 0 0 0];
A4 = [0 0 0 0.007 0 0];
A5 = [0 0 0 0 0.007 0];
A6 = [0 0 0 0 0 0.0061];
A = [A1;A2;A3;A4;A5;A6];
C = 1e9*inv(A); % Stiffness matrix

% angles
sint = sqrt(1-cost.^2);
sin2t = 2*sint.*cost;

% quasi shear wave in-plane

Y1 = ((C(1,1)-C(4,4))*(sint).^2+(C(4,4)-
C(3,3))*(cost).^2).^2+((C(1,3)+C(4,4))*sin2t).^2;

```

Appendix F (Continued)

```
Xp = C(1,1)*(sint).^2+C(3,3)*(cost).^2+C(4,4)-sqrt(Y1);
Stp = sqrt(2*rho)./sqrt(Xp);
Vtp = 1./Stp;

% quasi longitudinal mode in-plane

Xn = C(1,1)*(sint).^2+C(3,3)*(cost).^2+C(4,4)+sqrt(Y1);
Slp = sqrt(2*rho)./sqrt(Xn);
Vlp = 1./Slp;

% pure shear mode polaized normal to the plane
Stn = sqrt(rho./(C(6,6)*(sint).^2+C(4,4)*(cost).^2));
Vtn = 1./Stn;

velocity_matrix = [Vlp;Vtp;Vtn];

end
```

Appendix G

MATLAB codes used for calculations in chapter 5 &6

Electric field – velocity relation for two dimensional material under Thornber – Feynman formalism for 3D material:

```
hbar0=1.0545887e-27; % [erg-s]
c0=2.99792458e10; % [cm/s]
f=6.242e11; % conversion factor [erg] to [eV]
q0=4.80320420e-10; % elementary charge [ESU]
me = 9.10938356e-28; % Free Electron rest mass [gram]
kB = 1.38064852e-16; % [erg/K]
T = 300; % [K]
kBT = kB*T; % [erg]
wLO=591.0832; % LO phonon frequency in cm-1
w=2*pi*wLO*c0; % Phonon frequency in s-1
b= (hbar0*w)/kBT; % beta
%Eph=0.0699; % Phonon Energy [eV]
%b= (Eph)/kBT; % use this form for beta if Phonon
Energy is given
%-----
%Polaron Parameters

a=1.0224;v0=3.1123;w0=2.8676;x0=0.5*b*v0;
f=6.242e11; % conversion factor [erg] to [eV]
m0 = (v0/w0)^2; % ratio of polaron mass to electron effective
mass in lattice
m_eff=0.27;
m=m_eff*me; % me is the rest mass of electron
mp=m_eff*m0;% ratio of polaron mass to free electron rest mass
%-----
E0 = (0.5*a)*sqrt(b/pi)*(1/sinh(0.5*b));
A =1+(1-w0^2/v0^2)*((v0*b)/(2*sinh(0.5*v0*b))-1);
B=b*(w0^2/v0^2)*(((v0/w0)^2-1)/v0)*tanh(0.25*b*v0)+0.25*b);

q = @(x) integral(@(k)(sign(k).*exp(-
((b*k.^2)/(8*A))*((4*B)/b^2)-A)).*(exp(0.5*b)*exp((-0.5*b)*(x-
0.5*k-1./k).^2)+exp(-0.5*b)*exp(-b./(2*(x-0.5*k+1./k)).^2))),-
inf,inf);
fun =@(x) x.*q(x);

v = logspace(-2, 2,100);
n=length(v);
for i=1:n
    x=0:0.01*v(i):v(i);
    y=arrayfun(fun,x);
```

Appendix G (Continued)

```

E(i)= simpsons(y,0,v(i)/sqrt(A),3).*(E0./v(i).^2);

end

E1= E/2.75;
v1= v*0.418e16;

Fb=sqrt(mp)*(hbar0*w*f)^1.5*1e8*1e-3*E1;
Vr=sqrt(1/mp)*1e-8*(hbar0*w*f)^0.5*v1;
Eel= 0.5*m*m0*Vr.^2*f;

%
% PLoTting Velocity-Field

loglog(Vr,Fb,'LineWidth',2.0)
set(gca,'FontSize',26,'FontWeight','bold')
xlabel('V (cm/sec)','FontSize',26,'FontWeight','bold')
ylabel('eE (keV/cm)','FontSize',26,'FontWeight','bold')
title('CdSe','FontSize',26,'FontWeight','bold')
xlim([1e5 2.5e9])
ylim([1e0 1e3])
grid on
hold on
%}

Program for evaluation of variational parameters  $v_0$  and  $w_0$ 
%-----
% This program evaluates variational parameters: V0 and W0 for
plotting Thornber_Feynman Curves
%-----
a=0.2;%Frohlich Coupling Constant

% Expression of Ground state energy of polaron to be minimised
f = @(v,w) ((3*(v-w).^2./(4*v))-(integral(@(t)(pi)^-
0.5*a*v*( (w.^2.*t+((v.^2-w.^2)/v).*(1-exp(-v.*t))))).^-0.5.*exp(-
t),0,inf)));
x0 = [rand,rand];
[xmin, fval] = fminsearch(@(x)f(x(1),x(2)), x0);
% The above statement evaluates V0 and W0 and minimum value of
polaron ground stae energy
v0=xmin(1)
w0=xmin(2)
Emin=fval
mass_polaron=v0^2/w0^2

```

Appendix H

MATLAB codes used for calculations in chapter 7

Electric field – velocity relation for two dimensional material under Thornber – Feynman formalism:

```
% PLOtting Velocity-Field in SI Units

wLO = 1387.2;           % LO phonon frequency in cm-1
m_eff = 0.54;
einf = 4.97;           % Dielectric Const (High Freq)
e0 = 6.82;
T = 300;
%
[E_TF,V_TF] = TF_2Dloss(wLO,m_eff,einf,e0,T);
[idx] = find(E_TF == max(E_TF));
Vth = V_TF(idx);
Eth = max(E_TF);

subplot(1,2,1)
loglog(V_TF,E_TF,'LineWidth',3.0)
set(gca,'FontSize',15,'FontWeight','bold')
xlabel('V [cm/sec]','FontSize',15,'FontWeight','bold','Interpreter','latex')
ylabel('eE (KeV/cm)','FontSize',15,'FontWeight','bold','Interpreter','latex')
hold on

grid on

%
%% FGR
%
[E_FGR,Vel] = FGR_2Dloss_alt(wLO,m_eff,einf,e0,T);
[jj] = find(E_FGR == max(E_FGR));
VthF = Vel(jj);
EthF = max(E_FGR);

loglog(Vel,E_FGR,'LineWidth',2)

set(gca,'LineWidth',1)
set(gca,'FontSize',15,'FontWeight','bold')
xlabel('V [cm/sec]','FontSize',15,'FontWeight','bold','Interpreter','latex')
```

Appendix H (Continued)

```

ylabel('eE (KeV/cm)', 'FontSize', 15, 'FontWeight',
'bold', 'Interpreter', 'latex')
title('HfSe_2')
%legend('TF', 'FGR', 'location', 'best')
%}

%% Finding mobility in TF

E_field = E_TF(1:idx);
velocity = V_TF(1:idx);
mobility = mean(dydx(velocity, E_field*1e3));

Description of function TF_2D loss which computes energy loss in TF formalism
function [E_TF, V_TF] = TF_2Dloss(wLO, m_eff, einf, e0, T)

hbar0=1.0545887e-27; % [erg-s]
c0=2.99792458e10; % [cm/s]
f=6.242e11; % conversion factor [erg] to [eV]
q0=4.80320420e-10; % elementary charge [ESU]
me = 9.10938356e-28; % Free Electron rest mass [gram]
kB = 1.38064852e-16; % [erg/K]
% [K]
kBT = kB*T; % [erg]
w=2*pi*wLO*c0; % Phonon frequency in s-1
b= (hbar0*w)/kBT; % beta

%-----
%Polaron Parameters

a=alpha(wLO, m_eff, einf, e0);
[v0, w0]=VarParam_2D(a); x0=0.5*b*v0;
m=m_eff*me; % me is the rest mass of electron
m0 = (v0/w0)^2; % ratio of polaron mass to electron effective
mass in lattice
mp=m0*m_eff; % ratio of polaron mass to free electron rest mass

%-----

A =1+(1-w0^2/v0^2)*((v0*b)/(2*sinh(0.5*v0*b))-1);
B=b*(w0^2/v0^2)*(((v0/w0)^2-1)/v0)*tanh(0.25*b*v0)+0.25*b;
E02D = (0.25*a)*sqrt(b/pi)*(1/sinh(0.5*b))*(1/A);

```

Appendix H (Continued)

```

q2D = @(x,v) integral(@(k) (sign(k).*exp(-
((b*k.^2)/(8*A)).*((4*B)/b^2)-A)).*(exp(0.5*b)*exp((-
0.5*b)).*((v/A).*cos(x))-0.5*k-1./k).^2)+exp(-0.5*b)*exp(-
(0.5*b).*((v/A).*cos(x))-
0.5*k+1./k).^2)),0,inf,'ArrayValued',true);
fun2D = @(x,v) cos(x).*q2D(x,v);
f2D = @(v) integral(@(x) fun2D(x,v),0,2*pi);

v = logspace(-2, 1.6,5000);

E2D=arrayfun(f2D,v);

%

E1_2D= E02D*E2D/2.75;
v1_2D= v*0.418e16;
%{

Fb2D=sqrt(mp)*(hbar0*w*f)^1.5*1e8*1e-3*E1_2D; %KeV/cm
Vr2D=sqrt(1/mp)*1e-8*(hbar0*w*f)^0.5*v1_2D; %cm/sec

F_um = Fb2D*1e-1; %V/um

E_TF = Fb2D;
V_TF = Vr2D;

End

```

Description of function FGR_2Dloss_alt which computes energy loss by the electron in the purview of Fermi's golden rule:

```

function [E_loss,Vel] = FGR_2Dloss_alt(w_LO,m_eff,einf,e0,T)
hbar0=1.0545887e-27; % [erg-s]
c0=2.99792458e10; % [cm/s]
fx=6.242e11; % conversion factor [erg] to [eV]
q0=4.80320420e-10; % elementary charge [ESU]
m0 = 9.10938356e-28; % [gram]
kB = 1.38064852e-16; % [erg/K]

kBT = kB*T; % [erg]

pic2 = 2*pi*c0;

```

Appendix H (Continued)

```
m = m0*m_eff;
wLO= w_LO*pic2;
a = alpha(w_LO,m_eff,einf,e0);
b = hbar0*wLO/kBT;
Nq = 1./(exp(b)-1);
A1 = sqrt(2*m)/hbar0;
Emin = hbar0*wLO;
Emax = 5/fx;

CE = a*wLO*sqrt(hbar0*wLO)*(Nq+1);
CA = a*wLO*sqrt(hbar0*wLO)*(Nq);

fle = @(E,q)1./sqrt(1- (hbar0^2/(2*m*E)).*(0.5*q +
m*wLO./(q*hbar0)).^2);

fla = @(E,q)1./sqrt(1- (hbar0^2/(2*m*E)).*(0.5*q -
m*wLO./(q*hbar0)).^2);

itaue = @(E)CE*sqrt(1./E)*integral(@(q) fle(E,q)./q,A1*(sqrt(E)-
sqrt(E-hbar0*wLO)),A1*(sqrt(E)+sqrt(E-
hbar0*wLO)),'ArrayValued',true);

itaua = @(E)CA*sqrt(1./E)*integral(@(q) fla(E,q)./q,A1*(-
sqrt(E)+sqrt(E+hbar0*wLO)),A1*(sqrt(E)+sqrt(E+hbar0*wLO)),'Array
Valued',true);

En = linspace(Emin, Emax,8000);
%EnA1 = linspace(0, 0.99*Emin,8000);
%Emain = [EnA1,En];

ItauE = arrayfun(itaue,En);
%ItauA1 = arrayfun(itaua,EnA1);
ItauA2 = arrayfun(itaua,En);

Vel = sqrt(2*En/m);

E_loss = (ItauE-ItauA2)*(hbar0*wLO*fx*1e-3)./Vel;

End
```

Appendix H (Continued)

This function evaluates the variational parameters v_0 and w_0 for the two dimensional material

```
% INPUT: a = Frohlich Coupling constant
% OUTPUT: V0 and W0

function [V0,W0] = VarParam_2D(a)

%(w.^2*t./(2*v.^2))+(v.^2-w.^2)*(1-exp(-v*t))./(2*v.^3);

f = @(v,w) (0.5*(v-w).^2./v-
0.5*a*sqrt(0.5*pi)*integral(@(t)exp(-
t)./sqrt((w.^2.*t./(2*v.^2))+(v.^2-w.^2)*(1-exp(-
v.*t))./(2*v.^3)),0,inf));

x0 = [rand,rand];
[xmin, fval] = fminsearch(@(x)f(x(1),x(2)), x0);
% The above statement evaluates V0 and W0 and minimum value of
polaron ground state energy
V0=xmin(1);
W0=xmin(2);

End
```

Appendix I

MATLAB codes used for calculations in chapter 9

This program evaluates confined LO phonon discrete wave vectors, discrete phonon spectral density and confined LO phonon – assisted exciton creation rate corresponding to $n = 1$ mode.

```
clear

% GaAs Constants
hbar0=1.0545887e-27;    % [erg-s]
c0=2.99792458e10;      % [cm/s]
eps0 = 1;
[einf, e0, w0_LO, wTO] = MatParam(0);
einf = 10.9;
e0 = 12.9;
q0=4.80320420e-10;      % elementary charge [ESU]
eV=6.242e11;            % conversion factor [erg] to [eV]
a = 5.65e-8;
R = 3e-7; % Radius of QD
ae = R;
ah = ae/1.15; %[hole confinement length]
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% Reading the excel file which stores the data points of
dispersion relation
A = csvread('GaAs2.csv');
pic2 = 2*pi*c0;

k = A(:,1); % wave vector
w0 = A(:,2); % phonon frequency
%

% plotting data points obtained from neutron scattering
experiments
subplot(1,2,1)
plot(k,w0,'or','LineWidth',3)
grid minor
%}
hold on
% fitting 9th order polynomial
p = polyfit(k,w0,9);
x1 = linspace(0,1);
y1 = polyval(p,x1);
wLO = (2*pi*c0)*y1(1);
%
% Plotting the fitted curve
```

Appendix I (Continued)

```
plot(x1,y1,'LineWidth',1)
xlabel('Wave vector (2\pi/a)')
ylabel('Frequency (cm^{-1})')
title('Fitted')
legend('data points','curve fit')
set(gca,'FontSize',22,'FontWeight','bold')
%}
%
% Plotting fitted curve on second panel Fig. 1
subplot(1,2,2)
plot(x1,y1,'LineWidth',1)
hold on
xlabel('Wave vector (2\pi/a)')
ylabel('Frequency (cm^{-1})')
title('Confined modes')
set(gca,'FontSize',22,'FontWeight','bold')
%}
%%%%Determining confined mode wavevectors%%%%%%%%%%%%
a9 = p(1);
a8 = p(2);
a7 = p(3);
a6 = p(4);
a5 = p(5);
a4 = p(6);
a3 = p(7);
a2 = p(8);
a1 = p(9);
a0 = p(10);
B = a/(2*R);

n = 1:10;
%wq = y1;
wq =
(a9*(B*n).^9+a8*(B*n).^8+a7*(B*n).^7+a6*(B*n).^6+a5*(B*n).^5+a4*
(B*n).^4+a3*(B*n).^3+a2*(B*n).^2+a1*(B*n)+a0);

% Confined mode wave vector
% P.S: below is scaled wave vector
% The actual wave vector in cm^{-1} is obtained by multiplying
(2*pi/a)

qn = B*n; % confined scaled wave vector = (n*pi/R) / (2*pi/a)
%qnc = qn*(2*pi/a); % actual confined wave vectors
qnc = n*pi/R;
%figure(2)
plot(qn,wq,'s','MarkerFaceColor','r')
```

Appendix I (Continued)

```

ylim([230 300])
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

%%% Spectral density
%%% flm(k)
flm = sqrt(2*pi*hbar0*wLO*2/R).*sqrt(1/einf-1/e0);

r = linspace(0,R,1000);

Vq1 = -flm.*(2*q0/(pi*ae^3))*r.*(sin(qnc'.*r)./qnc').*exp(-
r.^2/ae^2);

Vq2 = flm.*(2*q0/(pi*ah^3))*r.*(sin(qnc'.*r)./qnc').*exp(-
r.^2/ah^2);
Vq = Vq1+Vq2;

for i = 1:10
    Mq(i,:) = trapz(r,Vq(i,:));
end

Jc = (1/hbar0^2)*abs(Mq).^2;

Jps = Jc*1e-12; %spectral density in ps^-1

figure(2)
stem(wq, Jps/pic2,'LineWidth',3)
xlabel('confined mode: Phonon frequency (cm^{-1})')
ylabel('Phonon Spectral Density (ps^{-1})')
%title('Confined modes: Phonon spectral density for GaAS QD
(radius = 3nm) ')
set(gca,'yscale','log','FontSize', 20)

%figure (3)
theta = linspace(0,pi/2);
ratio = tan(theta);
itau = (pi/2)*sin(theta).^2*Jps(1);
tau_ps = 1./itau;
plot(ratio, tau_ps,'--' , 'LineWidth',1)
ylabel('Phonon relaxation time (ps)','Interpreter','latex')
xlabel('$\hbar f/\Delta$', 'Interpreter','latex')
xlim([0 6])

```

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