Chapter 3

Thermopower and mobility in InN heterostructures

3.1 Introduction

Over the past few decades, the subject of extensive research has been electron transport in 2D semiconductor heterostructure systems, namely, QWs and heterojunctions, the favourite material system being GaAs/AlGaAs. Though the electronic properties of GaAs/AlGaAs are widely studied, in recent years, the potential of III–nitride heterostructures in high-temperature, high-frequency device applications has been realized. In literature, three nitride-based heterostructure systems, namely, GaN/AlGaN, InN/InGaN, AlN/AlGaN and InN/InAlN find frequent mention. One of the reasons for this interest has been their potential for use in microelectronic and optoelectronic devices such as high electron mobility transistors, LDs, LEDs [3.1–3.3]. However, these systems are characterised by imperfections namely, dislocations introduced during growth process, in the active material [3.3]. Systematic studies of the transport properties in heterostructures of these systems, with an inclusion of realistic

Part of the work presented in this chapter has appeared in

situations would not only throw more light on the interactions operative in it, but also pave the way for optimizing the potential of semiconductor heterostructures for better and faster devices.

The transport properties in 2D semiconductor heterostructure systems are often studied considering the 2DEG to be confined in QWs or HJs, with infinite barriers. Semiconductor QWs and HJs usually fabricated, with a thickness of a few monolayers and of particular barrier heights, are far from the idealized case of infinite barrier height. They are characterised by wavefunction penetration into the barrier layers. This barrier penetration is known to affect the transport properties of narrow QWs of finite barrier height significantly. In literature, the studies of transport properties considering penetration of wavefunction into barrier layers are deficient.

As stated in the previous chapters, thermopower is an interesting and important transport property to study in semiconductor quantum well heterostructures. Being sensitive to the composition, scattering mechanisms and structure of the system, it is known to shed much light on the interaction between electrons and phonons, impurities and other defects [3.4–3.9]. The thermopower (TP) of semiconductor QW structures, particularly of GaAs/AlGaAs system, has been studied extensively assuming the barrier height to be infinite [3.4]. However, there do not seem to be any investigation of TP of QW systems considering the finite confinement of 2DEG.

InN is one of the attractive candidates of III-V nitride semiconductors. It has a narrow bandgap, a small effective mass and superior electronic transport properties compared to other nitrides, namely, high low-field mobility, a peak drift velocity and strong overshoot effect. These distinctive properties make InN an interesting material for application in high-speed,
high-frequency, high-power electronic devices such as high electron mobility transistors [3.2].

In this chapter, we study the transport properties of 2DEG in InN based heterostructure systems. In section 3.2 we present, for the first time, investigation of influence of wavefunction penetration on acoustic phonon limited mobility and thermopower in finite barrier InN/InGaN QWs. Calculations of mobility considering all relevant scattering mechanisms in InN HJs are presented in section 3.3.

3.2 Acoustic phonon limited mobility and thermopower in finite barrier quantum wells

Carrier scattering considering barrier penetration effects on mobility has been investigated mostly in GaAs/AlGaAs [3.10–3.13]. Considering the 2DEG in a quantum well to be confined by finite barriers, Gold and coworkers [3.11] have studied the influence of finite barriers on transport properties. Nag and coworkers [3.12, 3.13] have investigated the influence in narrow quantum wells. They find that the changed form factor and effective mass and lead to values of electron mobility in narrow quantum wells significantly different from those in wide quantum wells [3.12]. Incorporating the finite barrier height and screened electron-phonon interaction, Suresha et al have analysed experimental energy loss rates data in GaAs/AlGaAs multiple quantum wells [3.14].

Here, incorporating the effects of wavefunction penetration, we present our investigations of mobility and thermopower. We give the theory developed for phonon drag thermopower in finite barrier quantum wells and illustrate our results for InN/In<sub>x</sub>Ga<sub>1-x</sub>N QWs. In the section 3.4 we also give the investigations of mobility in heterojunctions.
3.2.1 Theory

3.2.1.1 Wavefunctions and eigenvalues

We assume a 2DEG to be confined to move along the plane of a square symmetric quantum well of width $L$ and of barrier height $V$. The electron wave functions and energy eigen values are given by (see (1.20) and (1.21)) [3.11]

$$\psi_{nk}(r,z) = u_k(r)\xi_n(z)\exp(i\mathbf{k} \cdot \mathbf{r}) \quad (3.1)$$

and

$$E_n(\mathbf{k}) = E_n + \frac{\hbar^2 k^2}{2m^*} \quad (3.2)$$

where $\mathbf{r} = (x, y)$ and $\mathbf{k} = (k_x, k_y)$ are, respectively, the 2D position and wave vectors of the electrons with effective mass $m^*$. $\xi_n(z)$ is the normalized wave function of the $n^{th}$ electric subband with energy $E_n$. Due to the finite barrier confinement of electrons, say in the $z$ – direction, some part of the electron wave function penetrates into the barriers and decays exponentially. In this work, for simplicity, we assume the electrons to populate only the lowest subband ($n = 1$). The electron wave functions in the well (w) and barrier (b) regions are given by (see (1.22)) [3.11]

$$\xi_1(z) = \begin{cases} 
B_b \exp(ik_bz) & z \leq -L/2 \\
A_w \cos(k_wz) & -L/2 \leq z \leq L/2 \\
B_w \exp(-ik_bz) & z \geq L/2 
\end{cases} \quad (3.3)$$

where $k_w=2\alpha / L$, $k_b=2\beta / L$, and the normalization constants $A_w$ and $B_w$, are expressed as:

$$A_w=(2A_o/L)^{1/2} \text{ and } B_b=A_w \cos(\alpha) \exp(\beta), \text{ with } A_o = \left(1 + \frac{\sin(2\alpha)}{2\alpha} + \frac{(\cos(\alpha))^2}{\beta}\right)^{-1}.$$

The energy eigen values, expressed as (see (1.23))

$$E_1 = \frac{2\hbar^2 \alpha^2}{L^2 m_w}, \quad (3.4)$$

are determined for $0 < \alpha \leq \pi / 2$ from the transcendental equation:
\[(m_b/m_w)^{1/2}(C - \alpha)^{1/2} = \alpha \tan \alpha, \quad (3.5)\]

where, \(C = (m_w l^2 V / 2 \hbar^2)\), \(\beta = (m_b/m_w)\alpha \tan \alpha\), and \(m_w\) and \(m_b\) denote the masses of electron in well and barrier regions, respectively. For quantum wells with infinite barriers \(\alpha = \pi/2\) and \(1/\beta = 0\).

Equation (3.5) is a transcendental equation and its solution can be obtained using numerical methods. The energy eigen values thus obtained depend on physical parameters such as mass of electron, well width and barrier height, which characterize the penetration of wavefunction into the barrier layers.

### 3.2.1.2 Barrier height

One of the important parameters for the design and analysis of heterojunction and quantum well based electronic and optoelectronic devices, is the band offset. The band offset is a consequence of the difference between the bandgap energies of the two constituent semiconductors. The barrier height of quantum well formed has significant impact on the electron mobility. The properties of the barrier layer become important, when the electron energy eigenvalue is comparable in magnitude to the barrier height. The barrier height for electrons (holes) is set by the discontinuity in the conduction (valence) band offset, \(\Delta E_c (\Delta E_v)\).

The barrier height due to the conduction band offset is

\[V(x) = \Delta E_c(x) = E_c^b - E_c^w \quad (3.6)\]

where, \(E_c^b (E_c^w)\) is bottom of conduction band of material in the barrier (well). For Indium (In) mole fraction, \(x\) of a InN/In\(_x\)Ga\(_{1-x}\)N heterostructure, the difference in energy gaps of well and barrier materials is given by

\[\Delta E_c(x) = \left(E_g(\text{InN}) - E_g(\text{InN})\right)\text{InN/In\(_x\)Ga\(_{1-x}\)N heterostructure)}\]
From interpolation and taking an account of quadratic dependence of mole fraction of composition, the energy gap of In$_x$Ga$_{1-x}$N can be expressed as [3.1]

$$E_g(In_xGa_{1-x}N) = \left[xE_g(InN) + (1-x)E_g(GaN) - x(1-x)b_w\right]$$  \hspace{1cm} (3.7)

where $b_w = 1.4$, is bowing parameter. With, $E_g(InN) = 0.7eV$ and $E_g(GaN) = 3.38eV$, the, conduction band offset written as

$$\Delta E_c(x) = 0.6805 \left(1.4x^2 - 4.08x + 2.68\right).$$

From (3.5), it is clear that, the probability of barrier penetration of wavefunction characterized by $\alpha$ is determined by energy eigen value, which depends on the parameter C. The dependence of the physical parameters, through C, on the QW barrier height (indium content) is illustrated in figure 3.1.

![Figure 3.1](image_url)

**Figure 3.1:** Variation of the constant C as function of indium composition in InN/In$_x$Ga$_{1-x}$N QW.

An increase in the indium content in the barrier layers decreases the value of C. We notice that, for a given composition of indium in barrier layer there exist several combinations of
well width and barrier height which correspond to same wavefunction penetration into the barrier. This shows that, the extent of wavefunction penetration into barriers depends on well width and barrier height.

3.2.1.3 Momentum relaxation times and mobility

In the low temperature region of interest (T < 100K), the processes contributing to electron scattering are due to acoustic phonons and the imperfections in the specimen. Here, to demonstrate the barrier penetration effects due to intrinsic scattering mechanisms, we consider (as in ultrapure defect-free samples) the scattering to be due to only the acoustic phonons via deformation potential (DP) and piezoelectric (PZ) couplings. Assuming quasi-elastic scattering of electrons from bulk phonons the expression for the momentum relaxation time for screened electron– acoustical phonon scattering is given by

$$\tau_j^{-1}(E) = \frac{1}{4\pi^2\hbar\epsilon} \int_0^{2k} \frac{dq}{\sqrt{4k^2-q^2}} \left[ F(q_z) \right]^2 |C_j(Q)|^2 \Delta (E, E'), \quad (3.8)$$

where, $$\Delta (E, E') = \frac{N_Q[1-f^0(E+h\omega_Q)] - (N_Q+1)[1-f^0(E-h\omega_Q)]}{[1-f^0(E)]}$$, $$\hbar\omega_Q$$ being the energy of a phonon with wave vector $$Q = (q, q_z)$$ and $$N_Q$$ the phonon occupation number. The matrix elements, $$|C_j(Q)|^2$$ for electron–acoustic phonon interactions via deformation ($$j=\text{DP})$$ and piezoelectric ($$j=\text{PZ})$$ couplings are given by [3.15],

$$|C_{DP}(Q)|^2 = \frac{D^2Q}{2\rho u_l} \quad (3.9)$$

and

$$|C_{PZ}(Q)|^2 = \frac{(e\hbar h_4)^2}{2\rho Q} \left[\frac{A_l}{u_l} + \frac{A_t}{u_t}\right]. \quad (3.10)$$

where, $$D$$ is deformation potential, $$h_4$$ is piezoelectric constant and $$A_l$$ and $$A_t$$ are anisotropy factors.
The form factor in the overlap integral in (3.8) is expressed as
\[ F(q,z) = 2A_o \cos(\alpha) \left[ \frac{2\beta \cos(t) - t \sin(t)}{4\beta^2 + t^2} \right] + A_o \left[ \frac{\sin t}{t} + \frac{t \cos(2\alpha) \sin(t) - 2\alpha \sin(2\alpha) \cos(t)}{t^2 - 4\alpha^2} \right], \quad (3.11) \]

with \( t = qL/2 \). For quantum wells with infinite barriers, (3.11) reduces to
\[ F(q,z) = \left[ \frac{\sin t}{t} - \frac{t \sin t}{t^2 - \pi^2} \right]. \quad (3.12) \]

In equation (3.6) the screening function, \( \varepsilon(q) \), is given by [3.11]
\[ \varepsilon(q) = 1 + V_e(q) [1 - G(q)] X(q), \quad (3.13) \]
where, \( V_e(q) = (2\pi e^2/\kappa_s q) F_e(q) \), is electron–electron interaction potential, \( G(q) \) is local field correction and \( X(q) \) is Lindhard function in two dimensions. The electron–electron interaction form factor, \( F_e(q) \), is given by
\[ F_e(q) = \int_{-\infty}^{+\infty} dz \left| \xi_1(z) \right|^2 \int_{-\infty}^{+\infty} dz' \left| \xi_1(z') \right|^2 e^{-q|z-z'|}. \]

The total acoustic–phonon relaxation time \( \tau(E) \), obtained by Mattheissen’s rule:
\[ \tau(E) = \sum_j \tau_j^{-1}(E), \quad (3.14) \]
determines the acoustic phonon limited electron drift mobility:
\[ \mu = \frac{e \langle \tau(E) \rangle}{m^*}, \quad (3.15) \]
where, the average \( \langle \tau(E) \rangle \) is given by (2.29).

### 3.2.1.4 Thermopower

Thermopower, \( S \), under open circuit conditions, is defined (in chapter 2) by [3.4]
\[ E = S \nabla T, \quad (3.16) \]
where, \( E \) is effective electric field developed in the presence of temperature gradient, \( \nabla T \). The diffusion component of TP, obtained employing the Boltzmann transport formalism, is
\[ S_d = \frac{1}{eT} \left( \frac{\langle E \tau(E) \rangle}{\langle \tau(E) \rangle} - E_F \right). \quad (3.17) \]
where, the symbols are defined earlier in (2.29).
The general expression for the phonon drag TP, for 2D semiconductors systems, given in chapter 2, is [3.16]

\[ S_g = \frac{2|e|}{h k_B T^2} \sum_k \Sigma_q \frac{h \omega_q}{\sigma} f^o(E(k)) \left( 1 - f^o(E(k + q)) \right) P_q(k, k') \tau_p \left( \tau_q \nu_k - \tau_k \nu_k \right), \nu_p(Q) \]  \hspace{1cm} (3.18)

where, the symbols are defined earlier.

At low temperatures (T < 100K), phonon transport in 2D semiconductor systems is limited mainly by boundary scattering and considering the contributions from both longitudinal (l) and transverse (t) modes one can take \( \tau_p = \Lambda/v_s \), where \( v_s \) is the velocity of phonons of mode \( s \) \((\equiv l, t)\) and \( \Lambda \) is the phonon mean free path [3.16]. In the case of 2DEG confined in QWs of finite height, (3.18) can be expressed in the boundary scattering regime, as

\[ S_g = \sum_s S_{gs} \]  \hspace{1cm} (3.19)

where, we write,

\[ S_{gs} = \frac{|e| \tau_{ps}}{2 \pi^2 k_B T^2 \hbar} \sum_q \frac{h \omega_q f^o(E(k)) \left( 1 - f^o(E(k + q)) \right)}{\left( \frac{h^2 k_0}{m^*} \right)^2 \left( \frac{h \omega_q - \hbar^2 q^2}{2m^*} \right)^{1/2}} |C_j(Q)|^2 |F(q_z)|^2 N_Q \tau_k \nu_s \frac{q^2}{(q^2 + q_z^2)^{3/2}}. \]  \hspace{1cm} (3.20)

The form factor \( F(q_z) \), given by (3.11) and (3.12), takes into account the finiteness of the barriers.

### 3.2.2 Results and discussion

We illustrate the influence of barrier penetration of wavefunction of 2DEG on acoustic phonon limited mobility and thermopower for finite barrier narrow InN/In\(_x\)Ga\(_{1-x}\)N quantum wells, for 5<T<100K. The material parameters, characteristics of InN used in our calculations are given in table 3.1 [3.17] (see page 42). In quantum wells of InN/In\(_x\)Ga\(_{1-x}\)N system, the confining barrier height, which corresponds to the conduction band offset, is between 1.55eV for \( x = 0.1 \) and 96meV for \( x = 0.9 \). Recently, InN/In\(_x\)Ga\(_{1-x}\)N multiple quantum wells grown with \( x = 0.7, 0.8 \) and \( 0.9 \) have been employed for optical characterization [3.18, 3.19 and 3.20].
Table 3.1: Material parameters of InN [3.17]

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acoustic deformation potential, $D$ (eV)</td>
<td>7.1</td>
</tr>
<tr>
<td>Longitudinal phonon velocity, $v_l$ (m/s)</td>
<td>$6.24 \times 10^3$</td>
</tr>
<tr>
<td>Transverse phonon velocity, $v_t$ (m/s)</td>
<td>$2.55 \times 10^3$</td>
</tr>
<tr>
<td>Static Dielectric constant, $\varepsilon_r$</td>
<td>15.3</td>
</tr>
<tr>
<td>High frequency dielectric constant, $\varepsilon_\infty$</td>
<td>8.4</td>
</tr>
<tr>
<td>Optical phonon energy, $\hbar\omega_o$ (meV)</td>
<td>89.0</td>
</tr>
<tr>
<td>Mass density, $\rho$ (kg/m$^3$)</td>
<td>$6.81 \times 10^3$</td>
</tr>
<tr>
<td>Effective mass, $m^*$ ($m_o$)</td>
<td>0.22</td>
</tr>
<tr>
<td>Lattice constant, $a$ (Å)</td>
<td>3.545</td>
</tr>
<tr>
<td>Lattice constant along c-axis, $c$ (Å)</td>
<td>5.703</td>
</tr>
<tr>
<td>Piezoelectric constant, $h_{14}$ (V/cm)</td>
<td>$9.2 \times 10^4$</td>
</tr>
</tbody>
</table>

Among the nitrides, InN and its alloys with GaN are found to possess superior transport characteristics compared to GaN and find applications in a variety of heterostructure based optoelectronics devices. Recently, MBE grown InN/In$_x$Ga$_{1-x}$N nanowire heterostructures, (with $x > 50\%$) exhibiting high crystalline quality nearly defect-free (free of dislocations) and with strong carrier confinement have been realized [3.21]. We have performed calculations of mobility and thermopower using (3.15) and (3.19) for InN/In$_x$Ga$_{1-x}$N quantum wells, with $L = 10$nm for 0.9 and 0.6 which correspond to barrier heights $V = 96\text{meV}$ and $500\text{meV}$, respectively and for infinite barrier height, for $5 < T < 100\text{K}$. It may be noted that owing to the extension of the wavefunction into the barrier layers, the effective mass of the electron in barrier layer varies [3.12] with composition of barrier material as $m_b = (0.22 - 0.105x)$. In our calculations, we take $n_s = 1 \times 10^{16} \text{m}^{-2}$, for which the Fermi energy is $E_F = 22\text{meV}$ and the electrons confined to the lowest subband.
Figure 3.2: Energy dependence of \(\tau^{-1}\) due acoustic phonons for InN/In\(_x\)Ga\(_{1-x}\)N quantum well of width 100Å. Curve 1, 2, 3, 4 and 5 show \(\tau^{-1}\) for \(V = 96\text{meV}, 212\text{meV}, 346\text{meV}, 500\text{meV}\) and for infinite barrier approximation respectively. Dotted and dashed curves, in inset, depict respectively, the contributions of scattering rates due to deformation and piezoelectric interactions to total (curve 1) for quantum well with \(V=96\text{meV}\).

Figure 3.2, shows the energy dependence of the acoustic phonon limited relaxation rates for three quantum well barrier heights. Curves 1, 2, 3 and 4 represent variation of total rate \(\tau^{-1}(E)\) for \(V=96\text{meV}, V=212\text{meV}, V=346\text{meV}\) and 500meV, respectively. Curve 5 corresponds to infinite barrier height. The dotted and dashed curves in inset depict, respectively, the variations of contributions from the deformation potential and piezoelectric couplings to total (curve 1) for the InN/In\(_x\)Ga\(_{1-x}\)N quantum well with \(V= 96\text{meV}\). We notice that, the rates increase with increase in energy, \(E\). The dominant contribution to the total rate at lower energies is from piezoelectric interaction and for higher energies the contribution from DP interaction becomes important. An increase in barrier height from 96meV to 500meV
increases $\tau^{-1}(E)$ without modifying its behavior. The infinite barrier approximation (curve 5) is found to overestimate the rates. This dependence may be attributed to the inverse dependence of $\tau^{-1}(E)$ and to on $E$ changes in the values of the form factor and effective mass.

The variation of form factor, $F(q_z)$, given by (3.11) and (3.12), is shown in figure 3.3 for 96meV (curve 1), 212meV (curve 2), 346meV (curve 3) 500meV (curve 4) and curve 5 corresponds to infinite barrier height. It is seen that with increase in barrier height the form factor not only increases in magnitude but also changes in its dependence on $q_z$. These dependences are expected to be reflected in transport properties.
Figure 3.4: Temperature dependence of acoustic phonon limited mobility, $\mu$ in InN/In$_x$Ga$_{1-x}$N quantum well of width 100Å and $n_s = 1 \times 10^{16}$ m$^{-2}$. Curves 1, 2, 3, 4 and 5 depict, respectively the $\mu$ for $V=96$meV, 212meV, 346meV, 500meV and infinite barrier approximation. Inset: Dotted and dashed curves show contribution to total (solid curve) mobility due to deformation potential and piezoelectric interactions for quantum well with $V=96$meV.

Figures 3.4 shows the temperature dependence of acoustic phonon limited mobility for the five values of barrier heights considered: $96$meV (curve 1), 212meV (curve 2), 346meV (curve 3) 500meV (curve 4); curve 5 corresponds to infinite barrier height. The dotted and dashed curves in inset of figure 3.4 denote the contributions to total mobility (solid curve) from deformation potential and piezoelectric interactions to total mobility for $V = 96$meV (curve 1). We notice that, mobility decreases with increase in the temperature. Corresponding to the energy dependence of rates, the mobility is found to decrease sharply for $T < 30$K and slowly for higher temperatures. The dominant contribution to total mobility is from piezoelectric interaction. A comparison of curves 1, 2, 3, 4 and 5 shows that the mobility values decrease with increase in barrier height and that, infinite barrier approximation
underestimates the true mobility. This may be attributed to increase in the form factor with increase in the barrier height. It may be noted here that, although the weighted average of the effective masses in the well and in the barrier layers increases, the penetration of wavefunction has general effect of reducing the form factor, and the scattering probability. This reduces the mobility for the infinite well case [3.12].

Figure 3.5 shows temperature dependence of diffusion thermopower, $S_d$ for different barrier height QWs. Curves 1, 2, 3 and 4 depict $S_d$ for $V = 96\text{meV}$, $V = 212\text{meV}$, $V = 346\text{meV}$ and $V = 500\text{meV}$ barrier height QWs respectively. Curve 5 denotes $S_d$ under infinite barrier approximation. For the range of temperatures and parameters considered, $S_d$ shows almost linear temperature dependence. An increase of barrier height from 96meV to 500meV
Figure 3.6: Temperature dependence of acoustic phonon limited \( S_g \) in InN/In\(_x\)Ga\(_{1-x}\)N quantum well of width 100Å and \( n_s = 1 \times 10^{16} \) m\(^{-2}\). Curves 1, 2, 3, 4 and 5 depict respectively the \( S_g \) for \( V = 96\) meV, 212meV, 346meV, 500meV and infinite barrier approximation. An increase of barrier height increases the \( S_g \). This may be attributed to the dependence of overlap integral. Infinite barrier height approximation overestimates.

decreases \( S_d \) by 10\( \mu \)V/K at 100K. We have also performed calculations of \( S_d \) under infinite barrier approximation. The magnitude of \( S_d \) under infinite barrier approximation overestimates the diffusion component of thermopower.
Figure 3.7: Variation of thermopower, \( S (S_g + S_d) \) as function of temperature in InN/InGaN quantum well of width 100Å and \( \Lambda = 1000 \) Å with \( n_s = 1 \times 10^{16} \) m\(^{-2}\). Curves 1, 2 and 3 show the variation of \( S \) for quantum wells of 96meV and 500meV and infinite barrier heights, respectively. Dotted and dashed curves show \( S_d \) and \( S_g \) respectively for QW with \( V = 96\)meV.

With a view to study the effect of barrier penetration of wavefunction on thermopower, \( S \), we have performed calculations of both components \( S_d \) and \( S_g \) using equations (3.17) and (3.20) for three barrier heights. Figure 3.7 shows variation of thermopower as function of temperature. For the range of temperatures considered, the magnitude of \( S_d \) is small (~80μV/K at 100K) and its temperature dependence is almost linear. \( S_g \) is evaluated assuming the phonon mean free path, \( \Lambda = 0.1\)μm, a typical value of the size of quantum well samples. The variations of explicit contributions from \( S_d \) (dotted curve) and \( S_g \) (dashed curve) to total \( S \) (curve 1) for the quantum well with \( V = 96\)meV are also shown in figure 3.3. It is, found that, with increase in the barrier height, \( S_g \) increases significantly in magnitude implying its sensitivity to indium (In) composition. At low temperatures (\( T < 20\)K) \( S_g \) shows \( T^{2.55} \), and \( T^{2.39} \) dependences for
Figure 3.8: Variation of thermopower, $S (S_g + S_d)$ as function of temperature in InN/InGaN quantum well of width 100Å and $\Lambda = 100$ Å with $n_s = 1 \times 10^{16}$ m$^{-2}$. Curves 1, 2 and 3 show the variation of $S$ for quantum wells of 96meV and 500meV and infinite barrier heights, respectively. Dotted and dashed curves show $S_d$ and $S_g$, respectively, for $V = 96$meV.

$S$ = 100Å

$S_g$ = 100Å

$S$ (μV/K)

$T$ (K)

x = 0.6 and x = 0.9, respectively; For higher temperatures ($T > 40$K), $S_g$ is found to saturate. In infinite barrier approximation, (curve 3) $S_g$ shows $T^3$ dependence for lower temperature region. A comparison of curves 1, 2 and 3 shows that the total thermopower, $S$, is overestimated by 49% and 17%, respectively.

Figure 3.8 shows temperature dependence of $S$, calculated for $\Lambda = 100$Å. In this case, the magnitude of $S$ decreases by one order of magnitude and contribution from diffusion component becomes important at higher temperatures. The temperature dependence of $S$ is altered for $T > 80$K for compositions of indium, $x = 0.9$ (curve 1), $x = 0.6$ (curve 2) and for infinite barrier approximation (curve 3).
Figure 3.9: Variation of thermopower, $S (S_g + S_d)$ as function of temperature in InN/InGaN quantum well of width $L = 100\text{Å}$, $V = 96\text{meV}$ and with $n_s = 1 \times 10^{16} \text{m}^{-2}$. Curves 1, 2, 3 and 4 show the variation of $S$ for $\Lambda = 40 \text{Å}$, $\Lambda = 60 \text{Å}$, $\Lambda = 80 \text{Å}$ and $\Lambda = 100 \text{Å}$ respectively.

With a view to understand the sensitivity of $S$ to the structure of system, we have performed the calculations of $S$ for various values of phonon mean free path. Figure 3.9 shows variation of $S$ for different values of phonon mean free path. Curves 1, 2, 3 and 4 depict the variation of $S$ for $\Lambda = 40 \text{Å}$, $\Lambda = 60 \text{Å}$, $\Lambda = 80 \text{Å}$ and $\Lambda = 100 \text{Å}$ respectively. An increase of $\Lambda$ not only increases $S$, but also alters temperature dependence.

In this section we presented, a systematic study of the dependence of both components of TP on the barrier height of QWs. Calculations of temperature dependence of low temperature acoustic phonon limited $S_d$ and $S_g$ for InN/In$_x$Ga$_{1-x}$N QWs for various values of $x$, bring out the influence of the extension of wavefunction into the barrier. The effect is
significant in the case of $S_g$, which depends on phonon mean free path. The relative importance of $S_d$ and $S_g$ is discussed.

### 3.3 Mobility in InN heterojunctions

As discussed earlier, owing to lattice mismatch between active and substrate layers, InN-based heterojunctions are characterized by unintentional imperfections such as threading dislocations of large densities ($N_d \sim 10^8–10^{10} \text{ cm}^{-2}$) [3.2]. These structural defects, introduced during the growth processes are expected to play an important role in limiting the electron mobility. An investigation of mobility in InN HJs, therefore provides a means of assessing the relative importance of carrier scattering mechanisms operative in this system.

In literature, there exist some studies of mobility in bulk InN [3.22]. Recently, HJs of InN/AlN, InN/GaN and InN/InGaN have been realized [3.22-3.24]. Using ensemble Monte Carlo simulation method Polyakov and Schwierz [3.23] have studied the dependence of mobility of 2DEG in a gated InGaN/InN heterostructure as a function of electron concentration. In this section we present investigations of the mobility of the 2DEG formed at InN HJs. We consider all the relevant scattering mechanisms operative in the system and employ the Boltzmann transport formalism in the relaxation time approximation. Following Leburton [3.25] we obtain an expression for the relaxation time due to polar optical phonon scattering.

#### 3.3.1 Theory

##### 3.3.1.1 Wavefunctions and eigenvalues

We consider a 2DEG spatially confined along $z$-direction perpendicular to the interface at a HJ. The electron wavefunctions and the energy eigenvalues are given by (see (1.7) and (1.15)) [3.26]
and
\[
E_n(k) = E_n + \frac{\hbar^2 k^2}{2 m^*}
\] (3.22)

where \( r = (x, y) \) and \( k = (k_x, k_y) \) are, respectively, the 2D position and wave vectors of the electrons with effective mass \( m^* \). \( \xi_n(z) \) is the normalized wave function of the \( n^{th} \) electric subband with energy \( E_n \). We will, in what follows, assume that the electrons in the inversion layer at the HJ occupy only the lowest subband (\( n=0 \)) and that the confinement profile is described by Fang-Howard variational wave function (see (1.11)) [3.26]

\[
\xi_0(z) = \left( \frac{b^3 \varphi_{N}^2}{2} \right)^{1/2} \exp(-b z/2)
\] (3.23)

with \( b \), the variational parameter, given by (1.12).

### 3.3.1.2 Momentum relaxation times and mobility

For the wide range of temperatures – (4.2K < T < 300K) considered, the processes contributing to electron scattering are due to lattice vibrations and lattice imperfections. Here, we consider, the 2DEG formed at InN heterojunction to be scattered by remote impurities (RI), background impurities (BI), interface charges (IFC), interface roughness (IFR), dislocations via coulomb (DC) and strain (DS) fields, acoustic phonons via deformation potential (DP) and piezoelectric (PZ) couplings and polar optical phonons (POP).

The theory for momentum relaxation time for various scattering mechanisms using Fermi Golden rule is well developed. The expressions for momentum relaxation times due to remote impurities, background impurities, interface charges, interface roughness, and dislocations via strain and Coulomb are well known and given by [3.27]

\[
\frac{1}{\tau_{RI}(E)} = C_o \frac{\hbar^3 N_{RI}^{1/3}}{6k^2} \int_0^{2k} dq \frac{q^3}{P_o(q,b)(4k^2-q^2)^{1/2}},
\] (3.24)
where, \( N_{RI} \) is remote impurity concentration, \( N_{BI} \) is remote impurity concentration, \( N_{IFC} \) is interface charge density, \( \Lambda \) correlation length, \( \Delta \) the rms height, \( \Gamma(q) = (4 \pi e^2/k_s) \left(n_{depl} + n_s/2\right)\), \( q = 2k \sin(\theta) \), \( \rho_L \) is charge density, \( N_D \) is dislocation density, \( \Lambda^*(q) \) is screening potential, \( a_c \) is the conduction band deformation potential, \( b_e \) is Burger vector, \( \lambda \) is poisons ratio.

At any finite temperature scattering electrons from acoustic phonons is inevitable. The expression for momentum relaxation time due acoustic phonons via deformation potential and piezoelectric interactions is

\[
\frac{1}{\tau_{pf}(E)} = \frac{m^*}{\pi^2 \hbar^2} \int_0^\pi d\theta (1 - \cos(\theta)) \int_0^\infty dq \frac{1}{\epsilon^2(q,T)} \left| \chi_{pq}(q) \right|^2 \Delta(q),
\]

where,
$|C_j(Q)|^2$ matrix elements, for electron–acoustic phonon interactions via deformation ($j=\text{DP}$) and piezoelectric ($j=\text{PZ}$) couplings and $I(q_z)$ is overlap integral.

At room temperature, electron transport is found to be affected by polar optical phonons in InN heterojunctions. We have obtained an expression for momentum relaxation time due to polar optical phonons using the formation of Leburton [3.25]. The expression for momentum relaxation time is given by

$$\frac{1}{\tau^{e(a)}(E)} = \frac{\alpha \omega}{\pi} \left( N_Q + \frac{1}{2} \pm \frac{1}{2} \right) \sum \int_0^{\phi_{\text{max}}} \frac{I_{2D}(q_z^{(a)}(E,\phi))}{\sqrt{\frac{k}{\hbar \omega} (\cos(\phi))^2 + 1}} \, d\phi$$

(3.31)

where, $\phi$ is angle between $k$ and $q$ and $e(a)$ denotes emission(absorption) of phonons and Frohlich’s constant is $\alpha = \frac{1}{2\hbar \omega} \frac{e^2}{\sqrt{\epsilon/2m_0 \omega}} \left( \frac{1}{k_\omega} - \frac{1}{k_\sigma} \right)$.

The integral $I_{2D}$ is given by

$$I_{2D}(q(E,\phi)) = \int_{-\infty}^{+\infty} \frac{|F(q_z L_z)|^2}{q^2 + q_z^2} \, dq_z ,$$

$q_z^{e} = k \cos(\phi) \pm \sqrt{k^2 (\cos(\phi))^2 - \frac{2m_0 \omega}{\hbar}}$, $q_z^{a} = -k \cos(\phi) \pm \sqrt{k^2 (\cos(\phi))^2 + \frac{2m_0 \omega}{\hbar}}$, and

$\phi_{\text{max}} = \cos^{-1} \left( \sqrt{\frac{\hbar \omega}{E}} \right)$ and $q_0$ is forbidden.

The total momentum relaxation time $\tau(E)$, is obtained by Mattheissen’s rule:

$$\tau(E) = \sum \tau^{-1}_i (E)$$

determines the total mobility:

$$\mu = \frac{e \tau_i(E)}{m^*}$$

(3.32)

where $\tau_i$ is the relaxation time for the $i^{th}$ scattering mechanism.

3.3.2 Results and discussion

We have performed numerical calculations of mobility of 2DEG at InN/AlN HJs using (3.32), for parameters characteristic of InN (see table 3.1) [3.17]. The other parameters chosen are
Figure 3.10: Temperature dependence of mobility in InN/AlN HJs. Curves a, b, c, d and e represent component mobilities due to interface(IFR+IFC), dislocation(DC+DS), impurity(RI+BI), acoustic phonon(DP+PZ), and POP scatterings, respectively, with $N_d=10^8$ cm$^{-2}$. Curve 1 denotes total mobility. Curve 2 represents total mobility for $N_d=10^9$ cm$^{-2}$. The range of electron concentration considered ($n_s=1-20\times10^{12}$ cm$^{-2}$) ensures that Fermi energy lies well below the second electric subband energy.

Figure 3.10 depicts temperature dependence of mobility, $\mu$ calculated with $n_s=2\times10^{12}$ cm$^{-2}$. Curves a – e, show the variations of the individual components of mobility, when the electrons are scattered by IFR+IFC, DC+DS, RI+BI, DP+PZ and POP respectively. Curve 1 represents the variation of the total contribution to $\mu$ with $N_d=10^8$ cm$^{-2}$. The maximum value of mobility is $3.5\times10^4$ cm$^2$/Vs at 140 K. It is seen that $\mu$, for the various mechanisms, except...
Figure 3.11: Variation of mobility in InN/AlN HJs as function of electron concentration. Curves a, b, c, d and e, represent component of mobilities from POP, IFR+IFC, DC+DS, DP+PZ and RI+BI, respectively. Curve 1 depicts total mobility.

for acoustic and optical phonon scattering increases almost linearly with temperature. For low temperature region, we find the dominant component of μ to be due to IFR scattering, whereas optical phonons become important for T > 160 K. The acoustic phonon component is negligible. We find that at lower temperatures dislocation scattering via coulomb interaction is significant. Curve 2 shows the temperature dependence of μ calculated with N_d = 10^9 cm^-2. It is seen that not only the magnitude of μ decreases by about one order of magnitude at 4K but also its variation is altered.

Figure 3.11 shows the variation of μ as a function of n_s at T = 300K for N_d = 10^9 cm^-2. Curves a – e denote the component mobilities due to scatterings from POP, IFR+IFC, DC+DS,
DP+PZ and RI+BI, respectively. Curve 1 represents total $\mu$. For the range of $n_s$ considered, we find that $\mu$ decreases with $n_s$. For lower $n_s$, $\mu$ is determined by POP and DC scatterings, whereas for higher $n_s$, by IFR scattering. With increase in electron concentration, 2DEG pushed closer to interface and hence mobility gradually limited by interface roughness scattering. For the range of $n_s$ considered, impurities and acoustic phonons show weak dependence.

To conclude, we have presented detailed calculations of wide temperature range mobility of a 2DEG at InN heterojunction considering all relevant scattering mechanisms operative in system. The role and relative importance of the individual scattering mechanisms are discussed. We found that, at low temperatures and high electron concentrations, interface roughness scattering mechanism is dominant and for higher temperatures polar optical phonons limit the mobility. An increase of dislocation density not only reduces the mobility but also alters behaviour.

REFERENCES


3.21 Kai Cui, Saeed Fathololoumi, Md Golam Kibria, Gianluigi A Botton and Zetian Mi, Nanotechnology, 23, 085205 (2012)

3.22 D. Zanoto et al, phys. stat. sol.(c) 2, 3077 (2005)


