CHAPTER 2

Diffusion Thermopower due to Interface Roughness Induced Piezoelectric Scattering in Lattice Mismatched Semiconductor Quantum Wells
2.1 Introduction

Under the open circuit condition the carriers diffuse down the temperature gradient and set up an electric field, which opposes the motion of the carriers due to the temperature gradient. This phenomenon of production of an electric field due to temperature gradient is called thermoelectric effect or Seebeck effect. The thermoelectric properties have always played vital role in elucidating transport and scattering mechanisms in semiconductors and metals [2.1, 2.2]. They have made significant contributions in understanding their electronic structure and density of states. Seebeck coefficient, the electric field developed per unit temperature gradient, is often loosely referred as thermopower.

Thermopower, $S$, arises due to the interdependence of potential and temperature gradient in a system where no electric current flows. It is defined by

$$S = \frac{E}{VT}, \quad (2.1.1)$$

where $E$ is the electric field produced by temperature gradient $VT$. Thermopower studies are used as sensitive probes of transport mechanisms. $S$ depends on the sign of the charge carriers unlike electrical and thermal conductivities, which depend on its magnitude. Though scattering is central to many of the proposed explanations of the resistivity and mobility, these properties are of limited help to distinguish between different scattering mechanisms. On the contrary, thermopower is a very sensitive probe of the scattering mechanism and usually complementary to resistivity (as it arises from the energy derivative of the energy dependent conductivity).

There are two contributions to $S$. They are diffusion thermopower, $S^d$, and phonon drag thermopower, $S^g$. The origin of $S^d$ is as follows. Under a temperature gradient, electrons diffuse through the specimen, which leads to setting up an electric field. A state of equilibrium is established between electrons moved down the temperature gradient and electrostatic repulsion due to excess charge at the cold end.
Other one is phonon drag thermopower ($S^8$) arising due to flow of phonon wind dragging electrons due to electron-phonon coupling. Thermopower is rigorously studied in metals and semiconductors and is well documented [2.1, 2.2].

During last two decades there has been considerable interest in the study of thermopower of low dimensional electron systems and a great deal of experimental and theoretical has been carried out [2.3-2.5]. The better understanding of the electronic structure, density of sates and transport mechanisms is made in the structures such as Si-MOSFET and GaAs/GaAlAs heterojunctions. In these structures the conventional scattering mechanisms, which are responsible in limiting the mobility and thermopower, are due to remote impurity, background impurity, interface roughness, alloy disorder and phonons. Both experimentally and theoretically it is confirmed that at liquid helium temperatures $S^8$ is dominant and for temperatures < 0.5K $S^d$ dominates.

It is also observed that in a Si- MOSFET $S^d$ changes sign when $n_s$ is varied [2.3]. This has been explained due to the dominance of scattering by background impurities and interface roughness as electron concentration increases. However, no such change in sign of $S^d$ is observed in GaAs/GaAlAs heterojunction due to scattering mechanism [2.6].

Recently, there is growing interest in the study of transport properties of lattice mismatched InGaAs-based and other QWs. A full understanding of scattering mechanisms in lattice mismatched InGaAs based QWs is of interest as they have been widely used in electronic and optoelectronic devices. It is shown that the well known scattering mechanisms such as impurity doping, alloy disorder, surface roughness fail to describe the measured electron mobility in some lattice mismatched QWs viz., In$_{0.2}$Ga$_{0.8}$As/GaAs and In$_{0.15}$Ga$_{0.85}$As/Al$_{0.23}$Ga$_{0.77}$As [2.7, 2.8]. Recently, Quang et al [2.9] have proposed a new important scattering mechanism, which is due to a large fluctuating density of roughness-induced piezoelectric charges giving rise to their piezoelectric field. This is shown to be significant in limiting the electron mobility of real strained QWs with a well width of the order of or greater than 50 Å and is
predominant over surface roughness scattering when the well width is larger than 100 Å. The combination of these two provides a perfect explanation for the low temperature electron mobility measured in lattice-mismatched InGaAs-based QWs. This new mechanism is expected to be much more important in strained nitride heterostructures such as AlN/GaN in view of their large piezoelectric constants, since the piezoelectric mechanism is governed by piezoelectric coupling constant, besides lattice mismatch. It is also suggested that the scattering by a random piezoelectric field might be one of the main mechanisms limiting the low temperature hole mobility in lattice-mismatched Si/SiGe heterostructures [2.9].

In this work we study S^d in lattice mismatched QWs. Particularly, the S^d due to the new scattering mechanism i.e. roughness induced piezoelectric field is calculated and its significance is compared with respect to the surface roughness scattering. Numerical calculations and results are presented for In_{0.2}Ga_{0.8}As/GaAs and AlN/GaN QWs.

2.2 Diffusion Thermopower: Boltzmann Approach

The Boltzmann equation is set up for two-dimensional electron gas in an electric field, E, and temperature gradient, VT, and it is solved in the relaxation time approximation for the steady state distribution function of the electron. This distribution function is used to obtain current density J. In the open circuit condition, J=0, the electric field developed per unit temperature gradient is obtained to give diffusion thermopower S^d. It is expressed as [2.3, 2.10]

$$S^d = \left( -\frac{1}{|e|T} \right) \int_{0}^{\infty} \frac{(E_k - \mu)\sigma(E_k)(df^0/dE_k)dE_k}{\int_{0}^{\infty} \sigma(E_k)(df^0/dE_k)dE_k} ,$$  \hspace{1cm} (2.2.1)

where f^0 is the equilibrium Fermi-Dirac distribution, \(\sigma(E_k)\) is the energy dependent electrical conductivity and \(\mu\) is the chemical potential. It is important to note that
thermopower is related to the energy dependence of the electrical conductivity and its
sign does not simply follow from the charge of the carriers but also depends upon
variation of $\sigma(E_k)$ with $E_k$.

For degenerate electrons, Taylor expansion of $\sigma(E_k)$ about $E_F$ gives

$$\sigma(E_k) = \sigma(E_F) + \left( \frac{d\sigma}{dE_k} \right)_{E_F}(E_k - E_F)$$
$$+ \left( \frac{1}{2} \left( \frac{d^2\sigma}{dE_k^2} \right)_{E_F} \right) (E_k - E_F)^2 + ...$$

Terms only up to second orders are retained since $d\sigma^0/dE_k$ falls rapidly to zero in the
range $k_B T$ around $E_F$. Only those terms anti-symmetric in $E_k$ will contribute and so, the
equation for $S^d$ becomes

$$S^d = \int_{E_F}^{E_k} dE_k \left[ \frac{d\sigma}{dE_k} \right]_{E_F} (E_k - E_F)^2$$

In this equation the Fermi integral has the value $(n_0 k_B T)^2/3$. Hence, the equation for $S^d$
reduces to the famous Mott formula

$$S^d = -\frac{\pi^2}{3} k_B \frac{k_B T}{|e|} \left( \frac{d\sigma}{dE_k} \right)_{E_F}$$

$$= -\frac{\pi^2}{3} k_B T \left[ \frac{d}{dE_k} \ln \sigma(E_k) \right]_{E_F}$$

The energy dependent electrical conductivity is given by [2.3]

$$\sigma(E_k) = \frac{n(E_k)e^2 \tau(E_k)}{m^*}$$

with the electron number density $n(E_k)$, relaxation time $\tau(E_k)$ and electron effective
mass $m^*$. For a two-dimensional electron gas $n(E_k) \propto E_k$. Taking the energy
dependent relaxation time $\tau(E_k) \propto E_k^p$ [2.11] with the scattering parameter


\[ p = \left[ \frac{E_F}{\tau(E_F)} \right] \left[ \frac{d\tau(E_k)}{dE_k} \right]_{E_k = E_F} \quad (2.2.6) \]

the equation for \( S^d \) is put in the form

\[ S^d = -\frac{1}{3} (p+1) \frac{\pi^2 k_B^2 T}{eE_F}. \quad (2.2.7) \]

We mainly consider a 2DEG in a lattice mismatched finite height QW of width \( L \) made of zinc-blende structure material e.g., InGaAs based. At very low temperatures electrons are assumed to be only in lowest subband. In order to calculate low temperature \( S^d \) in these structures, we consider mainly the relaxation time due to surface roughness scattering and roughness induced piezoelectric scattering. The relaxation time is expressed in terms of the autocorrelation function of disorder [2.12]

\[
\frac{1}{\tau} = \frac{1}{(2\pi)^2 \hbar E_k} \int_0^{2\pi} dq \int_0^{2\pi} dq' \frac{q^2}{(4k^2 - q^2)^{1/2}} \langle \left| U(q) \right|^2 \rangle, \quad (2.2.8)
\]

where, \( q = (q, \theta) \) is the 2D wave vector in the x-y plane, \( \langle \left| U(q) \right|^2 \rangle \) is the autocorrelation function of a disorder and \( \varepsilon_s(q) \) is the static dielectric function. In the random phase approximation the dielectric function of the 2D electron gas is given by [2.12]

\[
\varepsilon_s(q) = 1 + V(q)[1 - G(q)] \chi^0(q)
\]

\[
= 1 + \frac{q_{TF} C \xi(q)}{q} \varepsilon_s(q) \chi^0(q) \quad (2.2.9)
\]

with the normalization constant \( C = (\sqrt{L/2}) b_{01} \), where \( b_{01} \) is given by equation (1.4.10), the inverse 2D Thomas-Fermi screening length is given by

\[
q_{TF} = \frac{2m^* e^2}{\varepsilon_s h^2} \quad (2.2.10)
\]
where \( \varepsilon_l \) is the dielectric constant of the system, neglecting a small difference in its values for the well and the barrier. The screening form factor \( F_s(qL) \) in equation (2.2.6) accounts for the extension of electron states along the growth direction defined by

\[
F_s(qL) = \frac{1}{C^4} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} |\xi(z)|^2 |\xi(z')|^2 e^{-q|z-z'|} \, dz'dz.
\]  

(2.2.11)

By means of equation (1.4.9) for the lowest subband, this may be written in terms of a function of the dimensionless variable \( y=qL \) as [2.9]

\[
F_s(y) = s_1(y) + s_2(y) + s_3(y)
\]

(2.2.12)

where

\[
s_1(y) = \left\{ \frac{2}{y} \left( 1 + \frac{\sin a}{a} \right) + \frac{y}{y^2 + 4a^2} \left[ 1 + \frac{2a \sin a}{a} + \sin 2a \right] \right\}
\]

\[
+ \left\{ \frac{1}{y} \frac{y \cos a}{y^2 + 4a^2} \right\} \sinh (y/2)
\]

(2.2.13)

\[
s_2(y) = \left\{ 8 \left( 1 + \cos a \right) \frac{e^{-y/2}}{(y+2b)^2} \left[ \frac{2a \sin a \cosh (y/2)}{(y^2 + 4a^2)} \right] \right\}
\]

\[
+ \left\{ \frac{1}{y} \frac{y \cos a}{y^2 + 4a^2} \right\} \sinh (y/2)
\]

(2.2.14)

and

\[
s_3(y) = 2 \left( 1 + \cos a \right)^2 \left[ \frac{e^{-y}}{(y + 2b)^2} + \frac{y - 2b}{2b (y^2 - 4b^2)} \right]
\]

(2.2.15)
where
\[ a = k_w L \quad \text{and} \quad b = k_B L \tag{2.2.16} \]
and \( k_w \) and \( k_B \) are given by equation (1.4.11) and the function \( G(q) = q/2(q^2 + k_F^2)^{1/2} \) is the Hubbard local field correction. \( V(q) \) is the electron-electron interaction, \( \chi^0(q) \) is the polarizability of the electron gas [2.12].

In a QW of finite barrier height \( V_0 \) for surface roughness scattering the autocorrelation function is given by [2.9, 2.12]

\[
\left\langle |U_{SR}(q)|^2 \right\rangle = \left( \frac{\pi^{1/2} \hbar^2 C^2 a^2 \Delta \Lambda}{m_z L^3} \right)^2 \exp \left( -\frac{q^2 \Lambda^2}{4} \right) \tag{2.2.17}
\]

where \( C \) is the normalization constant of the envelope wave function, \( \Delta \) is the roughness amplitude, \( \Lambda \) is the correlation length and \( m_z \) is the effective mass of the electrons along the growth direction.

For roughness induced piezoelectric scattering the autocorrelation function is shown to be [2.9]

\[
\left\langle |U_{PE}(q)|^2 \right\rangle = \left( \frac{3\pi^{3/2} \hbar^2 G A e_{11} C^2 \Delta \Lambda}{8e_1 c_{44}} \right)^2 F_{PE}^2(qL) \exp\left(-q^2 \Lambda^2/4\right) \sin^2 2\theta \tag{2.2.18}
\]

where \( e_{14} \) is the piezoelectric constant, \( e_{11} = (a_b - a_w)/a_w \) is the parameter defining the lattice mismatch in terms of lattice constants of well \( (a_w) \) and barrier \( (a_b) \). Here \( G = 2(K + 1) \frac{c_{11} - c_{12}}{c_{11}}, K = 2c_{12}/c_{11}, A = 2c_{44}/(c_{11} - c_{12}), \) with \( c_{11}, c_{12} \) and \( c_{44} \) as the elastic stiffness constants of the strained layer. \( F_{PE}(qL) \) is the dimensionless form factor for the piezoelectric field and it is given by Quang et al [2.9]

\[
F_{PE}(q, z; L) = \int_0^L e^{-q \sqrt{z^2 + (z' - z)^2}} dz. \tag{2.2.19}
\]
In simpler form it is given by

\[ F_{PE}(q, z; L) = \begin{cases} 
\frac{1}{2q}e^qz \left(1 - e^{-2qL}\right) & \text{for } z < 0 \\
e^{-qz} \left(1 + 2qz\right) - e^{-q(2L-z)} & \text{for } 0 < z < L \\
2qLe^{-qz} & \text{for } z > L 
\end{cases} \] (2.2.20)

On introducing a dimensionless form factor for the piezoelectric field as a function of the dimensionless variable \( y = qL \) we can write

\[ F_{PE}(y) = p_1(y) + p_2(y)\sin a + p_3(y)\cos a \] (2.2.21)

where

\[ p_1(y) = \frac{1 - e^{-2y} + 2ye^{-y}}{y + 2b} + \frac{3 + e^{-2y} - 2(y + 2)e^{-y}}{y} \] (2.2.22)

\[ p_2(y) = \frac{2a}{y^2 + 4a^2} \left[ 1 - e^{-2y} + 2ye^{-y} + 4 \frac{y^2 (1 + e^{-y})}{y^2 + 4a^2} \right] \] (2.2.23)

and

\[ p_3(y) = \frac{1 - e^{-2y} + 2ye^{-y}}{y + 2b} + \frac{y}{y^2 + 4a^2} \left[ 1 + e^{-2y} - 2(y + 1)e^{-y} + 2 \frac{(y^2 - 4a^2)(1 - e^{-y})}{y^2 + 4a^2} \right] \] (2.2.24)

It is interesting to note that for roughness induced piezoelectric scattering the autocorrelation function depends quadratically on the lattice mismatch parameter. Unlike other known scattering mechanisms it also depends on the polar angle of the wave vector \( q \).

It is to be noted that \((1/\varepsilon)\) of each of the mechanisms has to be multiplied by 2 as a QW has two interfaces.
2.3 Numerical results and discussions

We have calculated the scattering parameter $p$ of the energy dependence of the momentum relaxation time and the diffusion thermopower $S^d$ as a function of electron concentration $n_s$ and well width $L$. The calculations are carried out at temperature $T = 0.5$ K at which $S^d$ is expected to be the only contributor to the thermopower [2.3]. We assume that among the conventional scattering mechanisms, interface roughness is the dominant mechanism at very low temperature. We choose In$_{0.2}$Ga$_{0.8}$As/GaAs and AlN/GaN QWs to illustrate the role of roughness induced piezoelectric mechanism in $S^d$. The carrier concentrations and well widths are chosen such that the gas is degenerate and occupies only the lowest subband.

2.3.1 In$_{0.2}$Ga$_{0.8}$As/GaAs QW

We first discuss the results in In$_{0.2}$Ga$_{0.8}$As/GaAs QW. Following are the In$_{0.2}$Ga$_{0.8}$As parameters used: $m=0.058 m_0$, lattice constant $a=5.7252$ Å, $c_{11}=11.10 \times 10^{11}$ dynes, $c_{12}=5.32 \times 10^{11}$ dynes, $c_{44}=5.56 \times 10^{11}$ dynes, $\varepsilon_L=13.45$ and $e_{14}=-0.137$ C/m$^2$. Lattice constant of GaAs is 5.64191 Å. In Figure 2.1, $p$ versus $n_s$ is shown for the InGaAs/GaAs QW of width 100 Å with $\Delta = 5$ Å and $\Lambda = 50$ Å which are closer to the values $\Delta = 8.5$ Å and $\Lambda = 49$ Å used by Quang et al [2.9] to explain the observed mobility in the specimen of Lyo and Fritz [2.7]. Plots are shown separately for interface roughness scattering (dashed curve), roughness induced piezoelectric scattering (dotted curve) and for both the mechanisms together (continuous curve).

It is found from Figure 2.1 that $p$'s due to both the mechanisms exhibit similar behaviors as a function of $n_s$. We find that at $n_s = 1.0 \times 10^{10}$ cm$^2$, $p$ due to piezoelectric scattering is more negative ($\sim -1.4$) compared to the $p$ due to the interface roughness scattering ($\sim -0.8$). $p$ becomes less negative with the increase of $n_s$. The difference in $p$ value due to the two mechanisms decreases and becomes zero at particular $n_s$. 

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Figure 2.1: Plot of the scattering parameter $p$ of the energy dependence of relaxation time versus electron density $n_s$ in In$_{0.5}$Ga$_{0.5}$As/GaAs QW for $L=100\,\text{Å}, \Delta =5\,\text{Å}, \Lambda = 50\,\text{Å}$ at $T=0.5\,\text{K}$. The dotted curve represents the piezoelectric scattering, the dashed curve represents the surface roughness scattering and the continuous curve is due to both the mechanisms combined.

For further increase of $n_s$, $p$ becomes positive and the difference in $p$ values of the two mechanisms increases again. There are notable differences in the values of $n_s$, corresponding to each mechanism, at which $p$ becomes zero. For the range of concentration considered here $p$ due to piezoelectric mechanism and due to both the mechanisms combined is nearly same indicating the dominance of the piezoelectric mechanism. This is consistent with the mobility calculations of Quang et al. It is interesting to note that, for a set of values of $L$, $\Lambda$ and $\Delta$ considered piezoelectric scattering and hence the combined scattering give $p = -1$ for $n_s = 3.1\times 10^{10}\,\text{cm}^2$. On the other hand, surface roughness scattering is not showing $p = -1$ in the entire range of concentration.
Figure 2.2: Plot of $S^d$ versus $n_s$ in In$_{0.2}$Ga$_{0.8}$As/GaAs QW. The Parameters and the curves are same as in Figure 2.1.

In Figure 2.2, diffusion thermopower $S^d$ is shown as a function of $n_s$ for InGaAs/GaAs QW for $L = 100$ Å, $\Delta = 5$ Å and $\Lambda = 50$ Å for each mechanism and the overall $S^d$. The significant feature is that $S^d$ due to piezoelectric scattering and hence the total scattering shows the change in sign for $n_s < 3.1 \times 10^{10}$ cm$^{-2}$. For $n_s = 3.1 \times 10^{10}$ cm$^{-2}$, $p = -1$ and $S^d$ is zero. For $n_s > 3.1 \times 10^{10}$ cm$^{-2}$, $p$ is greater than -1 and $S^d$ remains negative for piezoelectric scattering and overall scattering. The diffusion thermopower due to surface roughness scattering remains negative over the range of concentration considered here as $p$ is always greater than -1. Thus the sign of thermopower depends on the $p$ value of the dominant mechanism and in turn on the carrier concentration. It may be recalled that $S^d$ observations of Ruf et al. [2.13] show change in sign of $S^d$ when Fermi energy crosses a subband.

The magnitude of $S^d$ is governed by $(p+1)/\varepsilon_F$ indicating that $S^d$ decreases with increasing $\varepsilon_F$. In case of piezoelectric scattering $(p+1)$ decreases with the increasing $n_s$ for $n_s < 3.1 \times 10^{10}$ cm$^{-2}$. This results in rapid decrease of $S^d$ with the increasing $n_s$ in
this concentration regime. For $n_s > 3.1 \times 10^{10} \text{ cm}^{-2}$, $(p+1)$ increases resulting in slow change in $S^d$. In the larger concentration region $p$ is almost constant and $\sigma_F$ is large leading to a negative but nearly constant very small value of $S^d$.

In Figure 2.3, $p$ is shown as a function of well width $L$ at $n_s = 1.0 \times 10^{10} \text{ cm}^{-2}$. Due to both the mechanisms combined $p = -1$ at $L = 65 \text{ Å}$ and $p > -1$ for $L < 65 \text{ Å}$ and $p < -1$ for $L > 65 \text{ Å}$. This behavior is attributed to the dominance of surface roughness scattering for $L < 65 \text{ Å}$ and the piezoelectric is dominant for $L > 65 \text{ Å}$. Interestingly, this leads to $S^d = 0$ at $L = 65 \text{ Å}$ and $S_d$ is negative for $L < 65 \text{ Å}$ and positive for $L > 65 \text{ Å}$ as shown in Figure 2.4. It may be noted that in Si-MOSFET change in sign of $S^d$ is only due to $n_s$ [2.3] whereas in this system $S^d$ changes sign due to variation in $L$ too. We also find that value of $L$ at which $S^d$ becomes zero shifts to higher value for larger carrier concentration but less than $3.1 \times 10^{10} \text{ cm}^{-2}$.

The diffusion thermopower $S^d$ calculations are also performed as a function of $\Lambda$ for $n_s = 1.0 \times 10^{10} \text{ cm}^{-2}$ and $L = 100 \text{ Å}$ and it is found to decrease monotonously slowly with the increasing $\Lambda$. For example, $S^d = 10.2 \text{ } \mu \text{V/K}$ for $\Lambda = 50 \text{ Å}$ and $\sim 4.4 \text{ } \mu \text{V/K}$ for $\Lambda = 200 \text{ Å}$. We also find that the $n_s$ value at which $S^d$ is zero shifts to lower values for larger $\Lambda$. For instance for $\Lambda = 150 \text{ Å} S^d = 0$ for $n_s = 1.8 \times 10^{10} \text{ cm}^{-2}$. 
Figure 2.3: Plot of $p$ versus $L$ in In$_{0.2}$Ga$_{0.8}$As/GaAs QW for $n_s=1\times10^{10}$ cm$^{-2}$, $\Delta =5\text{Å}$, $\Lambda = 50\text{Å}$ at $T=0.5K$. The dotted curve represents the piezoelectric scattering, the dashed curve represents surface roughness scattering and the continuous curve due to both the mechanisms.

Figure 2.4: Plot of $S^p$ versus $L$ in In$_{0.2}$Ga$_{0.8}$As/GaAs QW. The parameters and the curves are same as in Figure 2.3.
2.3.2 AlN/GaN QW

In AlN/GaN QW we use the following GaN material parameters: $m=0.22m_0$, lattice constant $a=4.52\text{Å}$, $c_{11}=25.3\times10^{11}\text{dynes}$, $c_{12}=16.5\times10^{11}\text{ dynes}$, $c_{44}=6.04\times10^{11}\text{ dynes}$, $\epsilon=10.4$, and $c_{14}=-0.5\text{C/m}^2$. Lattice constant of AlN is $4.38\text{Å}$. The calculations of $p$ (Figure 2.5) and $S^d$ (Figure 2.6) are presented as a function of $n_s$ for $\Delta=5\text{ Å}$, $\Lambda=50\text{ Å}$ and $L=100\text{ Å}$. We find that from the mobility calculations piezoelectric scattering is dominant over the entire range of $n_s$. For a carrier concentration $4\times10^{12}\text{ cm}^{-2}$ mobility is found to be $261\text{ cm}^2/\text{Vs}$ for the parameters chosen here.

![Graph of p versus electron density $n_s$ in AlN/GaN QW for $L=100\text{Å}$, $\Delta=5\text{Å}$, $\Lambda=50\text{Å}$ at $T=0.5K$. The dotted curve represents the piezoelectric scattering, the dashed curve represents the surface roughness scattering and the continuous curve due to both the mechanisms combined. In this figure and in the following figures dotted curve and continuous curve are coinciding due to dominance of piezoelectric scattering.](image)

Figure 2.5: Plot of $p$ versus electron density $n_s$ in AlN/GaN QW for $L=100\text{Å}$, $\Delta=5\text{Å}$, $\Lambda=50\text{Å}$ at $T=0.5K$. The dotted curve represents the piezoelectric scattering, the dashed curve represents the surface roughness scattering and the continuous curve due to both the mechanisms combined. In this figure and in the following figures dotted curve and continuous curve are coinciding due to dominance of piezoelectric scattering.

It may be noted that experimental low temperature mobility in a specimen with $L=50\text{ Å}$ and $n_s=4.8\times10^{12}\text{ cm}^{-2}$ is found to be $720\text{ cm}^2/\text{Vs}$ [2.14] which may be
obtained theoretically with $A = 110$ Å and $\Delta = 5$ Å. Our calculations also show surprisingly very low mobility $\sim 7$ cm$^2$/Vs for $n_s = 4 \times 10^{11}$ cm$^{-2}$. It may be due to the strong piezoelectric coupling in this system. Change in sign of $S^d$ is observed in this system also due to piezoelectric scattering ($p < -1$) for $n_s < 1 \times 10^{11}$ cm$^{-2}$. For $n_s > 1 \times 10^{11}$ cm$^{-2}$, $p > -1$ and $S^d < 0$. The diffusion thermopower due to piezoelectric scattering in AlN/GaN system is larger compared to InGaAs/GaAs system. We also find that for $n_s < 6 \times 10^{10}$ cm$^{-2}$ with $L = 100$ Å, $p < -1$ and $S^d$ is positive for surface roughness scattering.

![Graph](image)

**Figure 2.6:** Plot of $S^d$ versus $n_s$ in AlN/GaN QW. The parameters and the curves are same as in Figure 2.5.

In Figures 2.7 and 2.8 $p$ versus $L$ and $S^d$ versus $L$ are given for $n_s = 5 \times 10^{10}$ cm$^{-2}$. Over the entire range of $L$ considered piezoelectric scattering is dominant and $S^d$ is positive for all $L$ and the $n_s$ chosen here. For surface roughness scattering $p$ and $S^d$ dependence of $L$ for $n_s = 5 \times 10^{10}$ shows that $S^d$ changes sign at $L = 75$ Å and remains positive for $L > 75$ Å.
We observe that $\tau_{SR}^{-1} \sim m_z^{-2}$ and $\tau_{PE}^{-1} \sim e_1^2$ and $m_z (\text{GaN}) \sim 4m_z (\text{InGaAs})$, $e_1 (\text{GaN}) \sim 4 e_1 (\text{InGaAs})$, $(a_w - a_b) = 0.12$ in AlN/GaN and 0.08 in InGaAs/GaAs. Hence the dominance of piezoelectric scattering is expected in AlN/GaN system.

![Figure 2.7: Plot of p versus L in AlN/GaN QW for $n_s=5\times10^{10}$ cm$^{-2}$, $\Delta = 5\text{Å}, \Lambda = 50\text{Å}$ at $T=0.5K$. The dotted curve represents the piezoelectric scattering, the dashed curve represents the surface roughness scattering and the continuous curve is due to both the mechanisms combined.](image)

We would like to note that a recent measurement of thermopower in a p-type Si/Si$_{1-x}$Ge$_x$ has shown $p = -2.15$ for $T < 0.5K$ leading to negative $S^d$ around this temperature [2.15]. Further, at about 2.2K, $p$ increases to $-1$ making $S^d$ to pass through zero and $S^d$ becomes positive for $T > 2.2K$. Phonon drag thermopower $S^g$ is extracted from the measured total thermopower by subtracting $S^d$. The authors have used the phenomenological expression for $p$ to calculate $S^d$. Hence, we emphasize that precise knowledge of $p$ is essential in determining $S^d$ and $S^g$.
2.4 Conclusions

In conclusion, we have studied the scattering parameter $p$, of energy dependence of the momentum relaxation time and diffusion thermopower $S^d$ due to a new surface roughness induced piezoelectric scattering, besides the surface roughness scattering, in lattice mismatched QWs. Numerical calculations are given for $\text{In}_{0.2}\text{Ga}_{0.8}\text{As}/\text{GaAs}$ and $\text{AlN}/\text{GaN}$ QWs at $T=0.5\text{K}$. The piezoelectric scattering is dominating the electron scattering and the $S^d$ at larger well widths. Interestingly, $p$ is found to be not only the function of electron density but well width as well. The variation of $p$ is found to be significant. For lower electron density $p$ due to piezoelectric scattering is found to be less than -1 and hence $S^d$ changing the sign. Also, $S^d$ due to this mechanism and the overall changes sign at larger well widths. Experimental measurements of thermopower will be a better test to understand the importance of this new mechanism.

Figure 2.8: Plot of $S^d$ versus $L$ in AlN/GaN QW. The Parameters and the curves are same as in Figure 2.7.
References


