4.1 Introduction

In this chapter, the thermoelectric power of a two-dimensional hole gas in a GaAs-AlGaAs heterojunction has been estimated considering both diffusion and phonon drag processes. The study of thermoelectric power is important in understanding the physics of low-dimensional systems as it furnishes information about the band structure, the density of states (DOS) distribution and the various scattering mechanisms operative [1]. Thermoelectric power is of current interest in phonon absorption and emission experiments because it is a quantity which is very sensitive to the conduction mechanism, scattering, carrier type and anisotropy [2-4]. Extensive theoretical studies on thermopower of both one and two-dimensional electron gas systems supported by heterostructures have already been done [5-9]. Experimental determination of thermopower of low-dimensional electron gas systems has also been carried out in various laboratories [10]. In the following sections, the diffusion thermopower and the phonon drag thermopower of a two-dimensional hole gas confined in a GaAs-AlGaAs heterojunction have been presented.

4.2 Theory of Diffusion Thermoelectric Power

The Diffusion Thermopower arises due to the diffusive motion of the carriers in a temperature gradient. It is an intrinsic property of the hole or electron gas. It is dependent on the scattering rate and carrier mobility at any particular temperature. In the case of highly degenerate semiconductors, the diffusion thermopower is calculated by using the Mott formula [11]. It is
derived by using the simple case of independent electrons or holes in a parabolic and for which the mean free path is energy independent.

For intrinsic semiconductors, where the electrons have a much higher mobility in comparison to holes, the latter can be neglected. The diffusion thermopower can be written as

\[ S_d \approx \frac{\left( E_c - E_F \right)}{|e|T} \]

where the electrons have a thermal energy equal to \(-\left( E_c - E_F \right)\). \( E_c \) is the conduction band edge. This formula is simple but it cannot explain the positive thermopowers observed in many metals. The flaw is rectified by taking the proper average values. If \( \sigma(E) \) is the conductivity of the electrons in the energy level \( E_i \) in a conductor and \( \mu \) is the chemical potential then,

\[ S_d = \frac{-1}{|e|T} \sum_i (E_i - \mu) \sigma(E_i) \]

The result obtained by utilizing Boltzmann transport equation would then be,

\[ S_d = \frac{-1}{|e|T} \int_{E_F}^{\infty} (E - \mu) \sigma(E) \left( \frac{df}{dE} \right) dE \]

Here, the Fermi-Dirac distribution has been represented by \( f \). For degenerate electrons, the above equation may be approximated by expanding \( \sigma(E) \) using the Taylor series. This expansion is possible because \( df/dE \) falls rapidly to zero outside the range \( E_F \pm KT \). Further the terms anti-symmetric in
e will contribute while others cancel out. Only the first few terms in equation (4.3) contribute. This leads to the expression that is referred to as the well-known Mott formula. The thermopower given by Mott formula is

\[ S = -\frac{\pi^2}{3} \frac{K K T d \ln \sigma}{d \ln E_{F}} \]  

The sign of the thermopower does not arise simply from the charge of the carriers. The negative sign for electrons arises because \( \sigma(E) \) usually increases with \( E \). Due to the same reason, for holes, the sign of the thermopower is positive \([5]\).

In this thesis, the diffusion thermopower of the two-dimensional hole gas in a GaAs-AlGaAs heterojunction has been calculated by using the Boltzman transport equation and the constant density of states function. Nag \([12]\) has described this method in detail for bulk semiconductors. Since holes are the carriers in this case, the sign is properly chosen to be positive. The wave function describing the two-dimensional hole gas in a GaAs-AlGaAs heterojunction is the usual Fang-Howard wave function \([13]\) given in Chapter 3. It has been assumed that the holes occupy the ground state only and the system has been described in detail in section 3.2 of Chapter 3. The expression of diffusion thermopower for bulk semiconductors given by Nag \([12]\) has been modified for the two-dimensional hole gas under investigation.

The diffusion thermopower is usually denoted by \( S_d \). The expression is,

\[ S_d = (eT)^{-1} \left[ \langle E \tau \rangle \left( \tau^{-1} \right) - E_F \right] \]  

where \( \tau \) is the relaxation time and \( \langle \rangle \) is the average over the hole distribution function and \( E_F \) is the Fermi energy. The relaxation time is governed mainly by
the dominant scattering process. In this case, it is the background impurity scattering [14].

4.3 Theory of Phonon Drag Thermopower

In addition to diffusion thermopower, there is also another contribution to the total thermopower due to a net phonon momentum associated with the heat flow when a temperature gradient exists. The interaction of the phonons with the carriers then leads to the transfer of a fraction of this momentum to the carriers and gives rise to a resultant electric field. This effect is called phonon-drag thermopower and is denoted by \( S_x \). The calculation of phonon-drag thermopower is quite complicated as it requires a knowledge of the non-equilibrium phonon and hole distributions. Phonon drag thermopower of electrons in low-dimensional and bulk semiconductors has been calculated both in the presence and absence of magnetic fields [15-20]. The phonon drag thermopower of a two-dimensional hole gas in an AlGaAs-GaAs heterojunction at low temperatures and non-degenerate carrier distribution has been calculated in this thesis by using a simple formula after Smith and Butcher [18,19]. Their model has been suitably modified for holes as there are two subbands degenerate at \( k=0 \) and characterized by two different effective masses. These two subbands are formed by splitting of the four-fold degenerate valence bands due to spin orbit coupling. This has already been mentioned in earlier chapters.

In general, the phonon drag thermopower for holes can be written as [21]:

\[
S_x = \frac{2}{3} \frac{1}{N_e eT V} \frac{\tau_\perp}{2 \tau_{hp}} \left( \hbar \omega_\perp \right)^2 \sum_k f(k) \left( 1 - f(k + Q) \right)
\]

where \( N_e \) is the volume density of electrons or holes, the volume being denoted by \( V \), \( \omega_\perp \) is the frequency of the phonons with wave vector \( Q \), \( k \) is the two-dimensional wave vector, \( f \) is the carrier distribution function.
In the limit of nondegeneracy, it may be assumed that \( \left( \frac{\hbar \omega}{m} \right)_k^2 \approx 2m v_T^2 K T \) Also, \( f(k) \ll 1 \) and \( f(k + Q) \) can be omitted. In this case, the phonon drag thermopower for a two-dimensional hole gas is given by,

\[
S_g = \frac{m^* v_f^2 \langle \tau_p \rangle}{3qT \langle \tau_{ph} \rangle}
\]

where \( \langle \tau_p \rangle \) is the average phonon relaxation time excluding hole-phonon interaction and \( \langle \tau_{ph} \rangle \) is the average hole-phonon relaxation time due to the relevant scattering. The relaxation time for the relevant scattering is obtained by taking the weighted average [14].

The phonon drag thermopower has been calculated for both the piezoelectric as well as the deformation potential acoustic phonon scattering. The relaxation times for these are given in chapter 3.

4.4 Results and Discussions

The individual mobilities for the two-dimensional hole gas limited by the various scattering mechanisms have been calculated using effective masses as predicted by Ekenberg [22]. The choice of the effective masses is justified by the agreement of the theoretical mobility values with experimental data [14, 23]. This has been shown in the previous chapter.

For calculation of diffusion thermopower, the relaxation time for background impurity scattering is most significant. Variation of the diffusion thermopower with temperature is shown in Fig 4.1. It is seen that diffusion thermopower has a tendency to saturate at higher temperatures. But for low temperatures the variation is almost linear. This behaviour is similar to that for electrons [7, 24].

The phonon drag thermopower has been calculated for both piezoelectric and deformation potential acoustic phonon scattering. Fig 4.2 shows the
Fig 4.1. Temperature variation of Diffusion Thermopower
temperature variation of the phonon drag thermopower for these two scattering mechanisms. It is seen that the phonon drag thermopower for piezoelectric scattering is more pronounced than that for deformation potential acoustic phonon scattering since piezoelectric scattering has a greater influence on mobility at lower temperatures.

There is considerable disagreement in the values of the deformation potential constant obtained so far [5]. In bulk GaAs the value ranges between 7eV to 8eV while many studies for GaAs heterostructures yield values in the range of 11-16eV [5]. The deformation potential constant in the valence band is \((5/8)E_I\) where \(E_I\) is the deformation potential constant for the conduction band. A recent study by Nolte et al. [25] gives the value of the deformation Potential constant as 9.3eV. This gives the deformation potential constant for the valence band near about the value we have chosen for our calculation. Phonon drag thermopower is calculated using values of the deformation potential constant lying between 7-16eV. Comparisons were done using the extreme values. It is found that the values limited by acoustic phonon scattering increase with increase of the value of the constant but remains less significant even for the highest value of 16eV. Hence phonon drag thermopower for the two-dimensional hole gas present in AlGaAs-GaAs heterojunctions is primarily governed by piezoelectric scattering. This is shown in figure 4.2.

It has been suggested in a previous work [26] that deformation potential acoustic phonon scattering is the dominant mechanism and piezoelectric scattering has an insignificant contribution, contrary to our finding. Phonon drag thermopower studies can throw some light on this issue. Comparison of theoretical and experimental data, if available, can resolve the problem. However, the contribution of deformation potential acoustic phonon scattering, though less prominent, is in no way negligible.

Phonon drag thermopower has a strong dependence on the phonon mean free path which is usually of the order of the minimum specimen dimension [5]. However, it is strongly dependent on temperature. According to Smith and
Fig 4.2 Temperature variation of phonon drag thermopower with temperature for 1. deformation potential acoustic phonon scattering, 2. piezoelectric scattering.
Butcher [18-20], uncertainties in the value of the phonon mean free path introduces considerable discrepancies in the value of the thermopower. This has been demonstrated experimentally by Fletcher et al. [27]. In this thesis, the dependence of phonon drag thermopower on phonon mean free path has been studied. This is shown in Fig. 4.3. The phonon drag thermopower for piezoelectric scattering changes more rapidly with phonon mean free path than that for deformation potential acoustic phonon scattering.

Fig. 4.4 shows the temperature variation of the effective thermopower along with the contribution from diffusion and phonon drag components. Even at low temperatures, the diffusion thermopower is overshadowed by the phonon drag contribution. The total thermopower is therefore dominated mainly by the contribution from the phonon drag effect.

If experimental values of thermopower are available the uncertainties in the values of phonon mean free path and deformation potential acoustic phonon constant may be resolved by comparing the theoretical values of thermopower with the experimental data.
Fig 4.3 Variation of the phonon drag thermopower with phonon mean free path
Fig 4.4 Temperature variation of the effective thermopower showing the contributions from diffusion and phonon drag processes.
References

3 A M Guenault, J Phys F Met Phys, 1, 373 (1971)
9 X Zianni and P N Butcher, J Phys Condensed Matter, 6, 2713 91994)
11 N F Mott and E A Davis, Electronic Process in Nonequilibrium Materials (Oxford University, N Y), Ch2, (1971)
16 V V Karyagin, I I Lyapalin and V V Dyakin, Sov Phys -Semicond, 22, 954 (1988)
19 M J Smith and P N Butcher, J Phys Condensed Matter, 1, 4859 91989b)
22 U Ekenberg and M Altarelli, Phys Rev B, 32, 3712 (1985)
24 B Tieke, U Zettler, R Fletcher, S A J Weigers, A K Geim,
   (1987)
27 R Fletcher, J C Maan, K Ploog and G Weimann, Phys Rev B, 33,
   7122 (1986)