

THERMOELECTRIC PROPERTIES OF Si-BASED TWO DIMENSIONAL STRUCTURES

By

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**Thesis submitted in partial fulfilment
of the requirements for the award of
the degree of Doctor of Philosophy
by the University of Warwick**

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March 2000

ABSTRACT

This thesis is a report on experimental investigations of electrical and thermal properties of Si/Si_{1-x}Ge_x/Si normal and inverted modulation doped structures and delta doped Si layers grown by solid source Molecular Beam Epitaxy (MBE). If the grown Si layer is B-doped at some distance (as spacer) before or after the alloy layer, this remote doping induces the formation of a quasi two dimensional hole gas (2DHG) near the inverted (SiGe on Si) or normal (Si on SiGe) heterointerfaces of the Si/Si_{1-x}Ge_x/Si quantum well, respectively. Other types of samples measured were δ -doped Si (2DHG) and δ <Sb>-doped Si (2DEG) structures.

Low temperature magnetotransport measurements (down to 0.3 K and at the magnetic field up to 12 T in strength) were carried out on one inverted 2DHG structure. The hole effective mass was extracted from the temperature dependence of Shubnikov-de Haas oscillations.

The thesis mainly presents experimental and theoretical results of zero magnetic field thermoelectric power (thermopower) for two dimensional hole gas and electron gas samples in the temperature range 1.5 – 300 K. The results correspond well with Cantrell-Butcher phonon drag thermopower theory. The temperature dependence of the thermopower is explained both in terms of the effects of phonon drag and the enhancement of electron-phonon interaction. Another contribution to the thermopower is the diffusion thermopower at low temperatures. The diffusion thermopower has been obtained experimentally for temperatures varying between 0.5 K and 1.6 K. The thermal conductivity was measured by applying a temperature gradient through the samples. The measured values of the thermal conductivity corresponded with T^3 temperature dependence law at low temperatures due to the boundary conditions. The phonon mean free paths were calculated from the thermal conductivity data and were found to be in agreement with Casimir length at low temperatures.

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ACKNOWLEDGEMENT

First of all, I would like to thank my supervisors Prof. T.E. Whall and Prof. E.H.C. Parker for their valuable guidance throughout my studies. I am very grateful to Dr. O.A. Mironov for his everyday supervising, fruitful comments, proof reading of my work & his technical expertise throughout the experimental phase of my studies.

My thanks are also due to Dr. P.J. Phillips who has provided MBE grown samples that have been used in my experiments. I would also like to mention the late Prof. P.N. Butcher & Dr. M. Tsousidou for their contributions towards the theoretical calculations on Thermopower data. I would like to acknowledge R. Morris, T. Naylor & the mechanical workshop who provided vital technical support.

My thanks also go to C. Possanzini, S.M Olsthorn, and J.C. Maan from the High Field Magnet Laboratory for providing the low temperature Thermopower measurements in Nijmegen University, The Netherlands. To D.J. Robbins, A.C. Churchill & W.Y. Leong for supplying the 2DEG sample from the Defence Evaluation Research Agency, Electronics Sector Great Malvern. To R. Ferguson, Department of Electrical and Electronic Engineering, Imperial College of Science ,Technology and Medicine, London, for the preparations of the Au contact on 2DEG sample.

My greatest thanks go to my wife for her tremendous support and commitment, without which I could not have completed my studies. To my children to make me smile at the end of a long day and to both our parents, for their patience, encouragement and inspiration to excel in all we do. Also I thank to my friend Y.C.O. Chen for his help in computers. Finally, I would like to thank Kirikkale University and the Higher Education Committee of Turkey, who provided me with the scholarship award to complete this thesis.

DECLARATION

This thesis is the result of research carried out by the author in Department of Physics, University of Warwick and is submitted as partial fulfilment of the requirements for the award of the degree of Doctor of Philosophy. The work described here is all my own, except where acknowledged as otherwise in the text.

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- S. Agan, O.A. Mironov, T.E. Whall, E.H.C. Parker, M. Tsaousidou and P.N. Butcher, "Two dimensional phonon-drag thermopower in $\text{Si}_{0.87}\text{Ge}_{0.13}/\text{Si}$ (001) heterostructure grown by MBE" at press *Microelectronic Engineering*, **51-52** 527 (2000).
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- **S. Agan**, I.G. Gerleman, O.A. Mironov, T.E. Whall, E.H.C. Parker, M. Tsaousidou and P.N. Butcher, "Thermoelectric properties of two dimensional Si-based systems", CMMP'96 Condensed Matter and Materials Physics Conference. The University of York, 18-21 December 1996, York, UK.
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CHAPTER ONE

INTRODUCTION

There now exists a massive amount of literature on the electrical transport properties of low dimensional semiconductor structures. Technological advances have made possible the realisation of high quality two dimensional electron (2DEG) and hole gases (2DHG). Most of the experimental and theoretical works have concerned the conductivity tensors of such systems. However, a very large body of this thesis has accumulated on the corresponding thermoelectric properties. The thermoelectric properties have played an important role in the transport and scattering mechanisms in conductors. In the thesis, after a brief comment on Si/SiGe heterostructures and delta doped Si layers, diffusion and phonon drag thermoelectric power (or thermopower) is mainly discussed experimentally and theoretically.

1.1 Technological uses of Si/SiGe heterostructures

As a research topic, Si has retained its hold. There are considerable government funds and university interests in this area. Integrated optoelectronics is another promising research field for Si devices. Detectors and wave guides have been demonstrated and integrated SiGe and Si devices are possible (Soref, 1993).

The first SiGe chips announced today are designed for wireless communications and include low-noise amplifiers, power amplifiers and discrete transistors. They are aimed at mobile phones and other wireless equipment. Manufacturing costs are the key to SiGe's success, especially with advocates claiming that it is one fifth the cost of GaAs for equivalent performance. Smaller geometry of Si have contributed to a vast set of improvements. Integrated circuits are getting smaller, faster, cheaper and pack more transistors per square centimetre. A reduction in operating voltages means less power consumption and less heat dissipation, and higher switching speeds.

Silicon germanium (SiGe) technology now appears capable of delivering viable products that will benefit from its high speed and ease of integration with CMOS processes (Sadek and Ismail, 1995 and Parker and Whall, 1998). The main technological use for the 2DHG formed in a modulation doped Si/SiGe heterostructure is discussed in the fabrication of fast Field Effect Transistors (p-channel FETs) and is therefore likely to be in the first generation of SiGe FET technology (Whall and Parker, 1998). The principle underlying its operation are

similar to the well known Si-MOSFET (Metal Oxide Semiconductor FET) (Pearsall and Bean, 1986).

Because the effective mass of electrons in Si (2DEG) is smaller than the effective mass of holes in SiGe heterostructures (2DHG) theoretically a faster electrical response and better devices should be expected from a 2DEG. Technological and economic disadvantages could be overcome by integrating the 2DHG with silicon technology.

The current best room temperature mobilities in SiGe strained layer structures are $2600 - 3000 \text{ cm}^2/\text{V.s}$ for electrons (Nelson *et al.*, 1993) and $1400 - 1850 \text{ cm}^2/\text{V.s}$ for holes (König and Dämbkes, 1995) at carrier sheet densities of the order of 10^{12} cm^{-2} . The room temperature effective mobility of a MOS device is obtained from the drain conductance in the ohmic region (Lander *et al.*, 1997). But theoretical calculations indicate that substantially higher room temperature mobilities are possible in fully pseudomorphic Si/SiGe/Si heterostructures (Laikhtman and Kiehl, 1993) but improvements are needed in growth temperatures and doping techniques.

1.2 Modulation doped Si/SiGe heterostructures

This section describes why a 2DHG may form at an epitaxial Si/SiGe heterointerface. When $\text{Si}_{1-x}\text{Ge}_x$ is grown epitaxially on a (001) silicon substrate, the conduction bands are nearly at the same energy, there is a step in the valence band energy of 0.74 eV (People, 1984).

When two different semi-infinite semiconductor crystals are joined together it is called a 'heterojunction' in the semiconductor literature. The thin sandwich structure of undoped Si contains no carriers and it is called a nominally undoped quantum well. If the outer Si cap layer (~ 10 nm) of the quantum well is doped with acceptors (the Si:B doping spike), holes will be trapped just inside the SiGe layer. The accumulation of a sheet of holes at the interface gives rise to the triangular band shape (the potential well). The carriers can be quantum mechanically confined into two dimensions respectively near the lower (inverted) or upper (normal) interface corresponding to pre-or post-boron doping of the Si/SiGe/Si quantum well. The 2DHG produces an electric field mostly in the undoped region (called the "spacer" layer). A spacer layer of undoped Si between the doping layer for concentrations above 10^{17} cm^{-3} and the SiGe well further separates the carriers from the doping impurities and thus achieves very high mobility. This technique is called **modulation doping** (Butcher, 1993).

In the epitaxial growth of such structures, the doped layer is either grown before or after the alloy. The former case refers to an inverted modulation doped structure but the latter arrangement refers to the normal structure. Layer configurations of inverted and normal modulation doped structures are shown in **Figure 1.1(a) and (b)**.

The principle of forming a two-dimensional carrier gas at a semiconductor-semiconductor interface was first obtained in the III-V system and was quickly examined in the SiGe system. The first report of a 2DHG at a Si/SiGe heterointerface was made by People *et al.*, (1984). A 2DEG can be

formed in a Si/SiGe system by using strain to increase the conduction band offset between the Si and the SiGe alloy. A useful feature of modulation doped systems is that the 2DHG does not freeze out even at very low ($T \rightarrow 0$ K) temperatures in contrast with simple doped structures (**Figure 1.1 c**).

The carriers are confined in the direction perpendicular to the layer and are constrained to move within it. **Figure 1.2** gives a schematic band diagram of a 2DHG Si/SiGe/ (001) Si modulation doped heterostructure. However, for the devices used in this work, the thickness (spread of the wave functions) of the 2D charge carrier layers are only ~ 5 nm for SiGe 2DHG (Emeleus, 1993), and ~ 8 nm for 2DHG Si delta boron doped structures (Krasovitskii *et al.*, 1995), even though they are confined to a layer whose thicknesses are macroscopic (30 nm for SiGe, and 375 nm for delta boron doped Si).

1.3 SiGe strained layers

Silicon (Si), germanium (Ge), and SiGe have a diamond structure (fcc lattice) with two atoms per basis. Si, Ge and SiGe have indirect band gaps and the bandgap of unstrained SiGe alloys are Si-like up to a Ge concentration of about 85% (Abstreiter, 1996). The atoms of Si and Ge are arranged randomly on the available lattice sites. Due to the symmetry of the fcc lattice, there are six band minima that located in the (100) direction of the Brillion zone for Si. In the conduction band, valley minima can be represented by ellipsoids of energy with simple **E** vs. **k** relations. For example in Si and for the [100] valley we get:

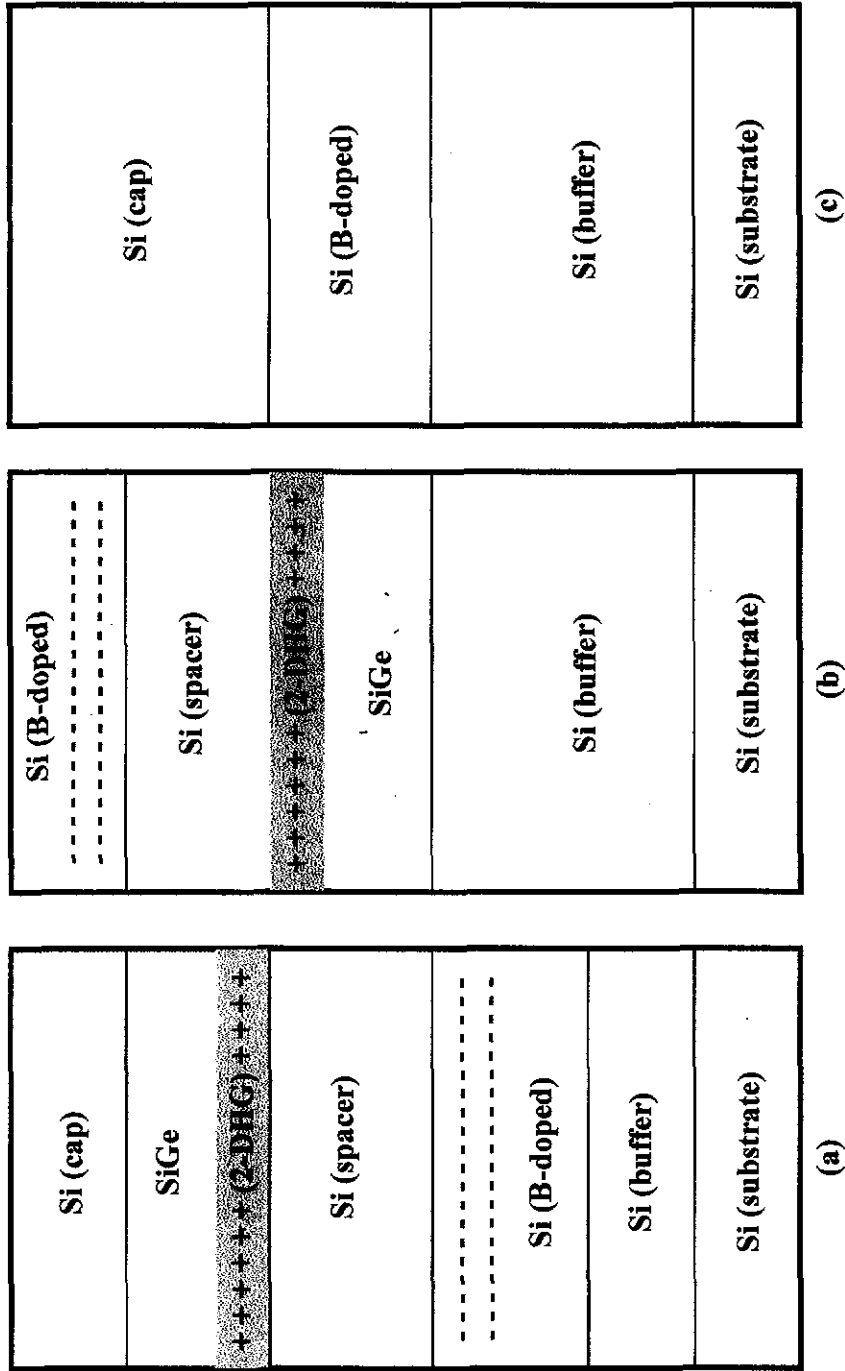
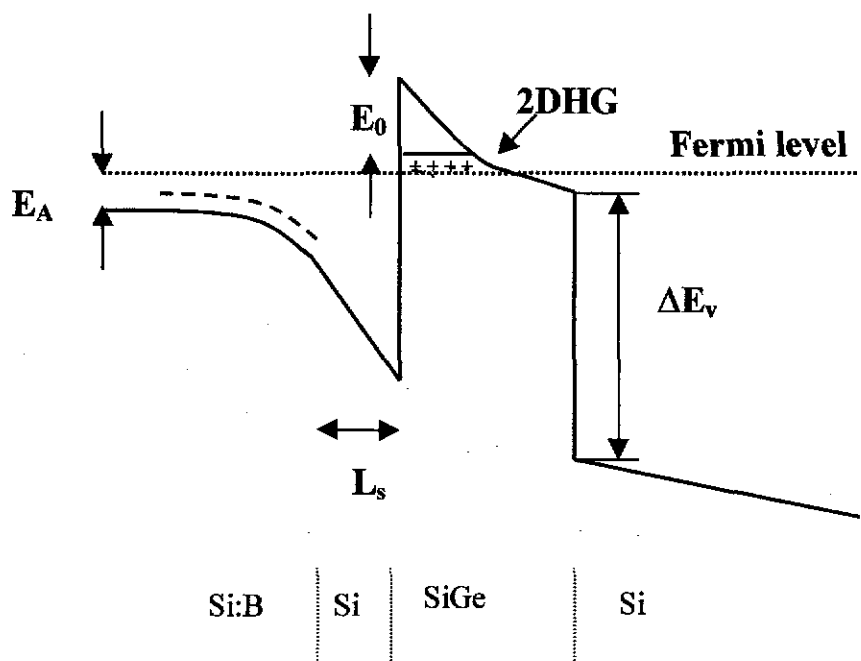


Figure 1.1: Schematic diagram of layer sequence and charge distribution (at $T \rightarrow 0\text{K}$) of (a) an inverted MD, (b) a normal MD, and (c) a simple B-doped structure (not to scale)

Figure 1.2: Schematic valence band edge diagram of 2DHG Si/SiGe/ (001) Si heterostructure. E_A is the boron activation energy in Si, E_0 the lowest lying 2DHG energy level, L_s the dopant set-back distance and ΔE_v is the valence band offset energy.



$$E(\mathbf{k}) = \frac{\hbar^2 k_z^2}{2m_t^*} + \frac{\hbar^2 (k_x^2 + k_y^2)}{2m_l^*} \quad (1-1)$$

where the m_t^* and m_l^* are effective masses of the four; transverse valleys ($m_t^*=0.19 m_0$) in the z-direction and another longitudinal mass for the remaining two valleys ($m_l^*=0.98 m_0$) in the x-y plane of $\mathbf{k}$ -space (Sze, 1981).

The lattice constant of Ge is 4.2% larger than that of Si. Epitaxial growth technologies have been developed which make possible the growth of coherent Si/Si_{1-x}Ge_x/Si structures, where the in-plane SiGe lattice spacing exactly matches that of Si. The central feature of Si/SiGe hetero-epitaxy is the lattice mismatch between Si and alloy materials, such that strain is accommodated in the epilayers. A critical thickness also exists which, if exceeded, will be accompanied by relaxation (**Figure 1.3**). The growth of SiGe on Si was first accomplished by Kasper, Herzog and Kibbel, (1975) using solid source molecular beam epitaxy (SS-MBE).

Valence band $E-\mathbf{k}$ dispersion relationships for strained SiGe quantum well structures have only been calculated for some cases (Ekenberg *et al.*, 1987). **Figure 1.4** shows the splitting of the light hole (LH) and heavy hole (HH) and confinement in a Si/Si_{0.5}Ge_{0.5} heterostructure (Ekenberg *et al.*, 1987). **Figure 1.5** shows the effect of strain on the valence band (O'Reilly, 1989). Quantum confinement produces a ladder of energy eigensates for each $|J, \pm M_J\rangle$ valance subband. In the Si/SiGe/Si sandwich structure, the compressive strain lifts the valance band degeneracy, reduces heavy hole mass and the band splitting

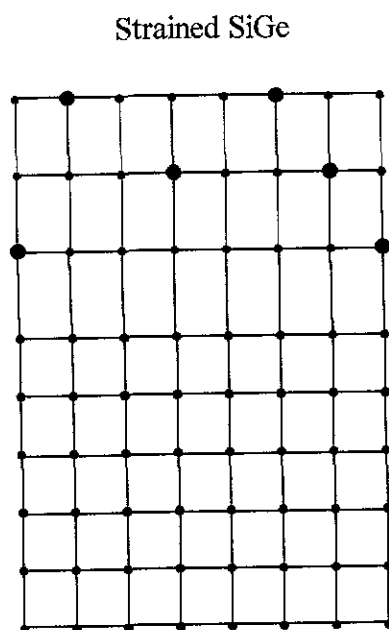
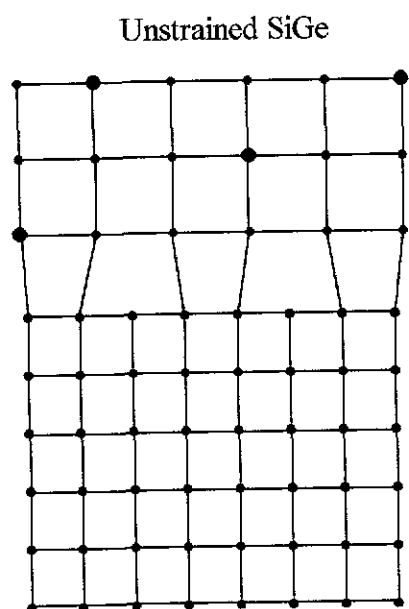
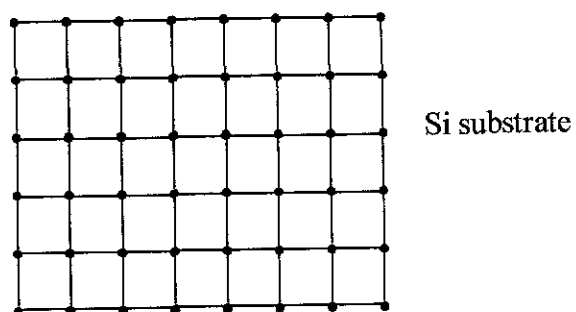
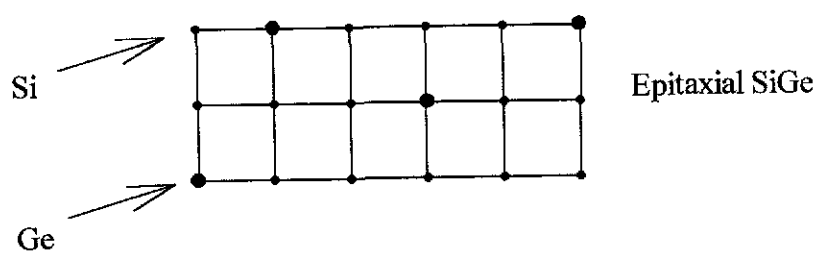
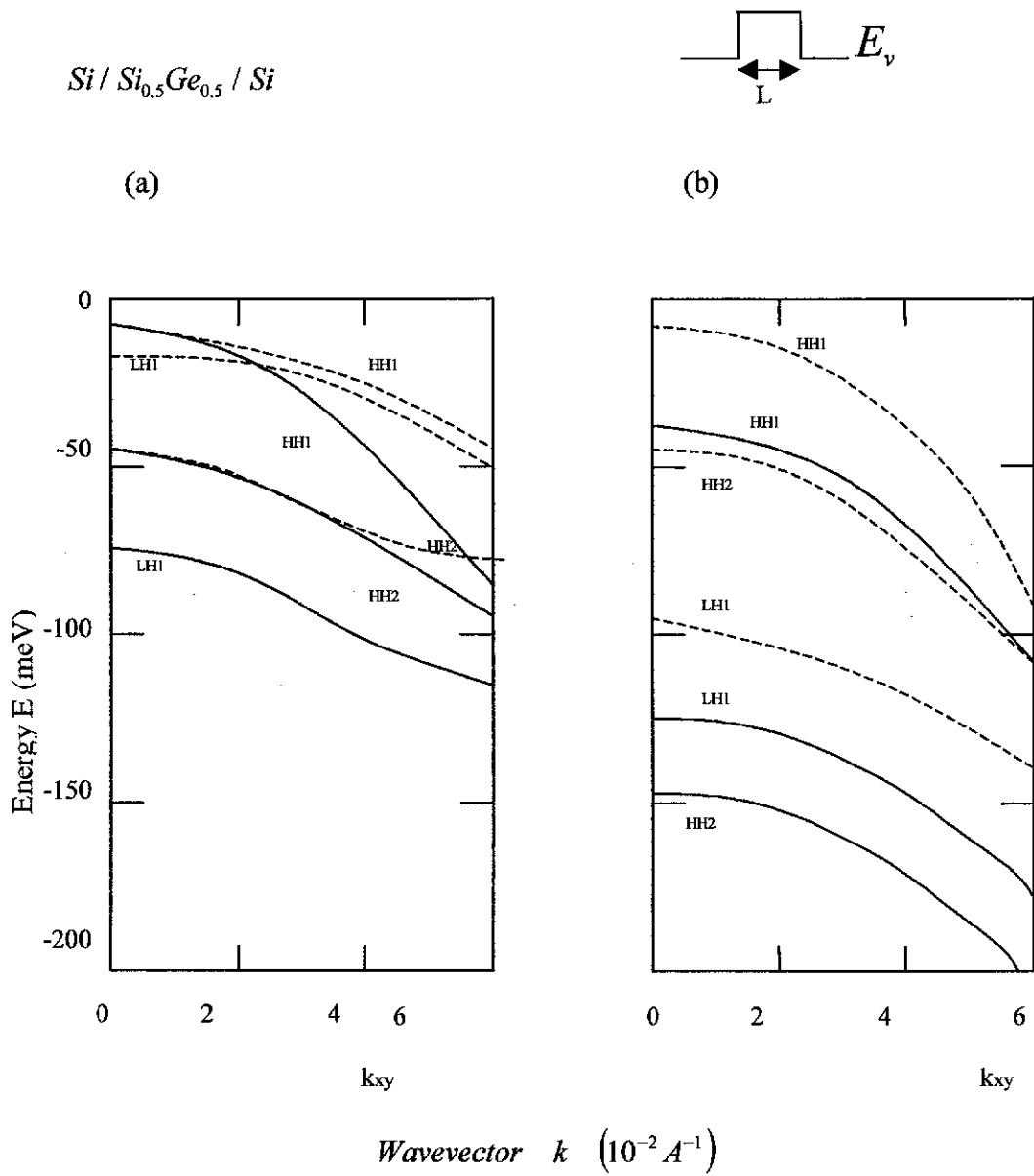


Figure 1.3: A schematic representation of the compressive strained in commensurate layers of SiGe grown on Si.

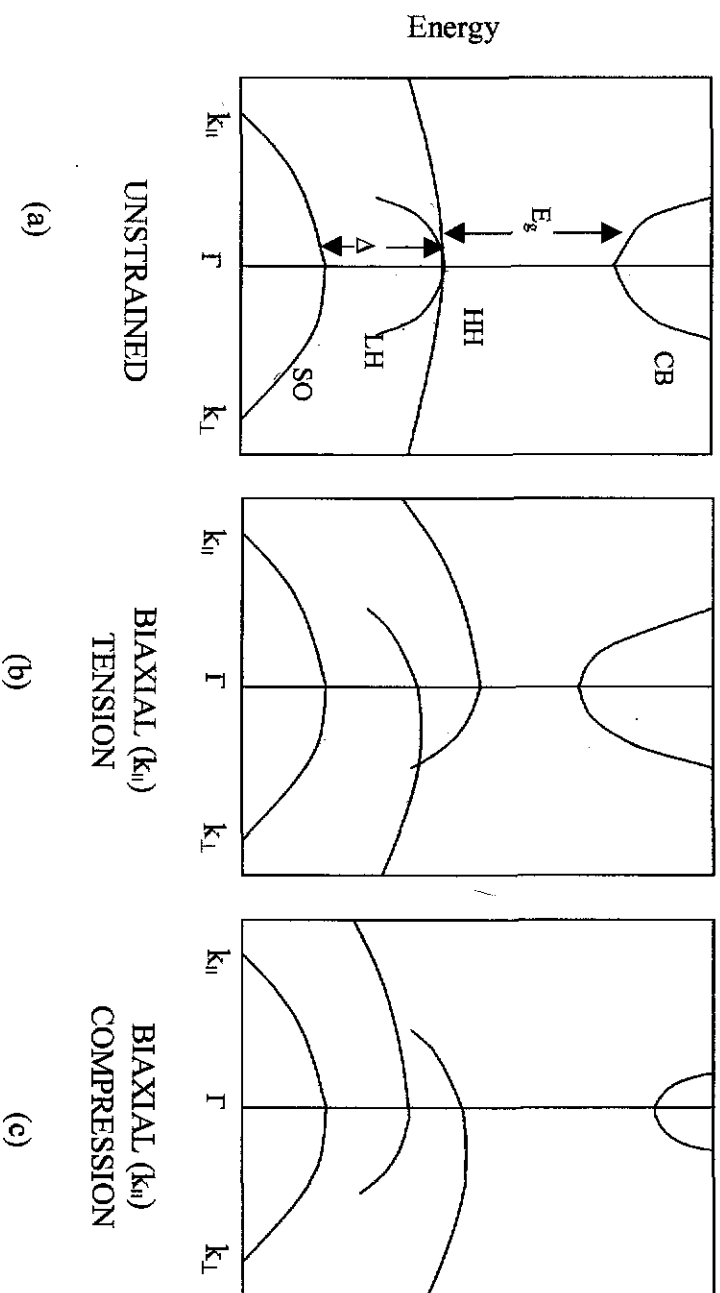
Figure 1.4: Effect of (a) biaxial compression and (b) confinement on valence band
 (After Ekenberg *et al*, 1987)



$L = 10 \text{ nm}$ {
 --- UNSTRAINED
 ____ STRAINED

STRAINED {
 --- $L = 10 \text{ nm}$
 ____ $L = 5 \text{ nm}$

Figure 1.5: (a) A schematic representation of the band structure of a unstrained direct-gap tetrahedral semiconductor. The light-hole (LH) and heavy-hole (HH) bands are degenerate at the Brillouin zone centre Γ and the spin-split-off (SO) band lies Δ lower in energy. The lowest conduction band (CB) is separated by the band-gap energy E_g from the valence bands. (b) Under biaxial tension, the hydrostatic component of the tension reduces the mean band gap, while the axial component splits the degeneracy of the valence band maximum and introduces and anisotropic valence band structure, with the highest band being light along the strain ($k_{\parallel}$) axis and comparatively heavy perpendicular to that axis (along $k_{\perp}$). Note that there is an ambiguity in the choice of notation which leads us to use here $k_{\parallel}$ for the direction perpendicular to the strain axis, $k_{\perp}$ lies in the growth plane and hence is perpendicular to the growth and strain direction. (c) Under biaxial compression the mean band gap increases and the valence splitting is reversed so the highest band is now heavy along the strain axis ($k_{\parallel}$) and comparatively light along $k_{\perp}$ (After, O'Reilly, 1989).



promotes enhanced carrier mobilities in the two dimensional hole gas (2DHG) (Whall, 1997). Stable strained layer structures have been successfully processed for device applications SiGe on Si. **Figure 1.6** shows energy electron bands in the Si MOS inversion layer. The fundamental properties of bulk Si and Ge semiconductors are listed in **Table 1.1**.

Table 1.1 Fundamental properties of bulk (un-strained) Si and Ge semiconductors

Semiconductor Material	Si	Ge
Lattice constant (Å)	5.431	5.657
Band gap (eV)	1.17	0.74
Electron Effective mass (m^*/m_0)	$m_l^* = 0.97 m_0$ $m_t^* = 0.19m_0$	$m_l^* = 0.16 m_0$ $m_t^* = 0.16m_0$
Hole Effective mass (m^*/m_0)	$m_{HH}^* = 0.5 m^*$ $m_{LH}^* = 0.16 m^*$ $m_{so}^* = 0.234m_0$	$m_{HH}^* = 0.3 m_0$ $m_{LH}^* = 0.04m_0$ $m_{so}^* = 0.095m_0$
Quantum States	$ 3/2, \pm 3/2\rangle$ $ 3/2, \pm 1/2\rangle$ $ 1/2, \pm 1/2\rangle$	$ 3/2, \pm 3/2\rangle$ $ 3/2, \pm 1/2\rangle$ $ 1/2, \pm 1/2\rangle$

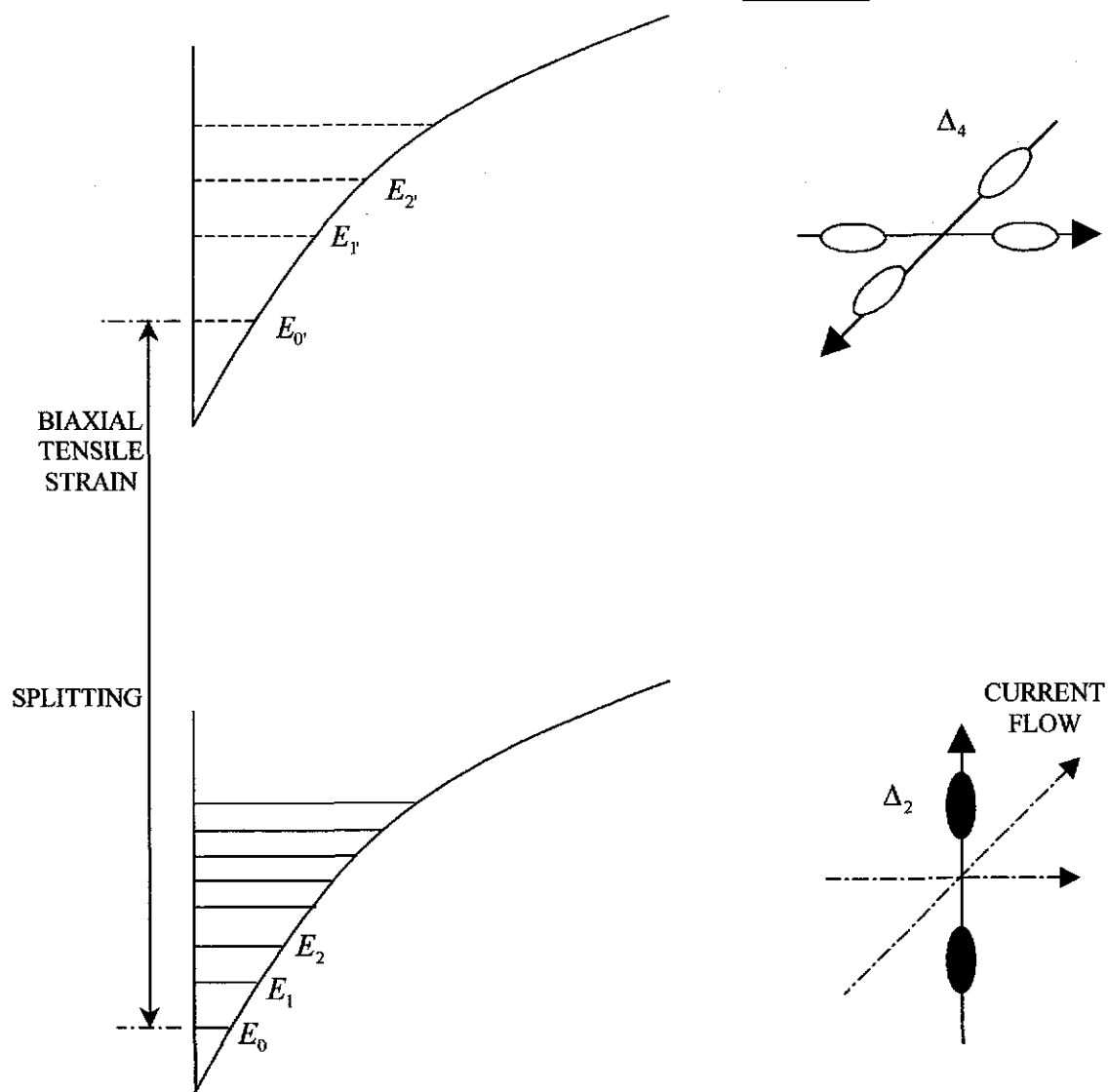
In two dimensional systems the effective mass approximation can be used for electrons/holes in the plane although where effective mass, m^* , is anisotropic the correct value for the appropriate crystal direction must be used. The effective

Figure 1.6: Energy electron bands in Si MOS inversion layer.

UNSTRAINED



STRAINED



mass of a carrier depends on the energy band it occupies, the momentum of the carrier, and the direction in the crystal field. In most cases, the effective masses of the carriers are less than m_0 , additionally they behave differently from the classical particles. One can obtain the effective mass from:

$$\frac{1}{m^*} = \frac{1}{\hbar^2} \nabla^2 E(k) \quad (1-2)$$

thus, for the parabolic shaped band edge the narrower the parabola, the smaller the effective mass.

A linear averaged method has been used to estimate the effective mass for bulk (un-strained) $\text{Si}_{1-x}\text{Ge}_x$ alloy from the bulk Si and Ge. The heavy hole mass at the band edge is approximately $m_{HH}^* = 0.46 m_0$ for $x=0.2$ (Chang *et al.*, 1994 and Whall *et al.*, 1994). At low temperatures, the carriers comprising the 2D gas occupancy for the ground (heavy-hole) subband only, are confirmed by an examination of SdH oscillations in the magnetoresistance of the samples (Sadeghzadeh, 1998).

1.4 Delta B and Sb doped layers in silicon

Recently, interest in the study of so-called delta (δ) layers, which represent atomic thickness conducting layers of foreign atoms (donors or acceptors) in a pure semiconducting crystal matrix, has increased considerably (Cashiering, 1996). Typically the dopant sheet is buried some tens of nanometres below the surface of the thin film and is popularly known as a δ -layer. Normally, these atoms are randomly distributed in space, so there is a high degree of

disorder (Whall, 1992). The delta layer is often grown in an intrinsic semiconductor as a doping layer. An n-type δ - layer in Si is illustrated in **Figure 1.7** (Ploog, 1987). Donors are located in an atomic monolayer of the (001) oriented Si host material, and the ionised donors provide a continuous positive sheet of charge. Here E_F is Fermi energy and E_0, E_1, E_2 are size-quantized energy levels for electrons inside symmetrical quantum-well. The fractional δ -doped coverage in the (001) plane can reach several percent. The impurity charge distribution n_s can be described mathematically by the Dirac delta function whose width is infinitely narrow (Schubert, 1996). At high temperatures, carriers will be excited into the conduction band and charge transport will be 2D if the potential well is narrow enough (Challis, 1992).

Two phenomena make the concept of δ -doping different from other 2D carrier systems. First, even at moderate δ -doping concentrations, the electrons populate several subbands. The sheet density of impurity atoms determines the number of size quantized subbands and their filling. The mobilities of charge carriers are strongly dependent on the number of the subband. The nature of the subband filling and the mobilities of charge carriers were the object of initial studies of δ -layers (mainly of $\delta\langle\text{Si}\rangle$ -layers in GaAs) (Koenraad *et al.*, 1993 and Panaev *et al.*, 1993). The second difference is the considerable delocalization of the carriers in the doping plane, i.e. the electronic states are spread out, of the some distance either side of the ionised donors which define the centre of the potential well.

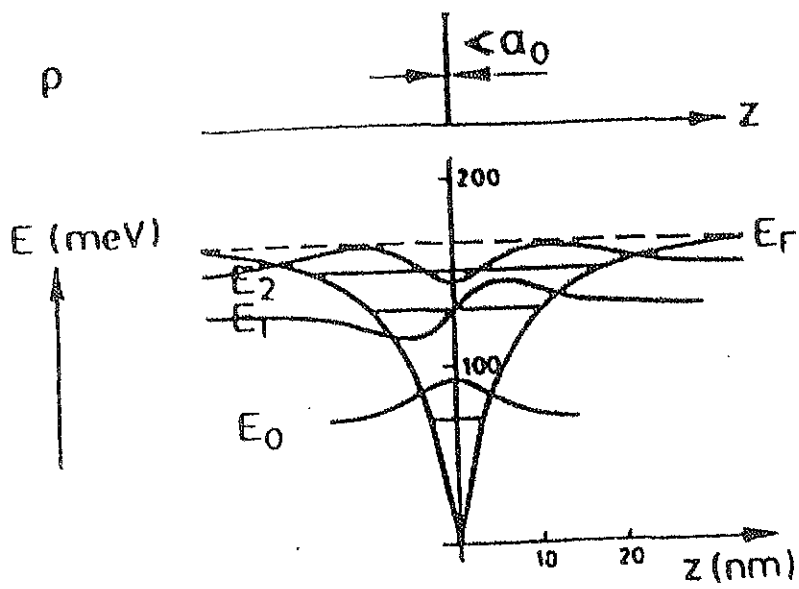


Figure 1.7: Schematic illustration of n-type δ -doping in Si.

The electronic structure is qualitatively, as well as quantitatively, different for semiconductors with an anisotropic band structure, such as Si or Ge. These semiconductors have constant energy surfaces shaped like rotational ellipsoids with longitudinal and transverse effective masses. The confinement of a free-carrier gas occurs along one spatial dimension (Gossmann and Schubert, 1993).

Many characteristics of semiconductor structures are related to potential fluctuations, such as the mobility of free carriers or the luminescence linewidth of doped structures. These characteristics can be optimised by using the δ -doping technique. If it was possible to place the doping atoms in an ordered, non-random arrangement, the carrier mobility would increase. The transport mobility of the electrons/holes is lower in δ -layers than in modulation doped heterojunctions because of the impurity atoms which formed the δ -layer. However, δ -layers are distinguished for an important and valuable feature: they allow an arbitrary density of two-dimensional electrons at very low sheet density values ($\approx 10^9$ - 10^{10} cm⁻²). The conductivity in the δ -layer is of "hopping" type, to very high values ($\approx 10^{14}$ cm⁻²) which realizes metallic conductivity. This feature of δ -layers provides a unique possibility for studying the effect of the concentration of two-dimensional electrons on relaxation and interaction of electrons in a two dimensional electron gas and on the character of the transition from the metallic to hopping conductivity. For δ <Sb>-layers in silicon, this transition occurs in the range of 0.01 monolayer (ML) of Sb atoms to 0.05 ML

in the δ -layer, which corresponds to the electron densities $6.7 \cdot 10^{12}$ to $3.35 \cdot 10^{13}$ cm^{-2} (van Gorkum, Nakagawa and Shiraki, 1989).

1.4.1 The literature on delta doping

The first reported growth of δ -layers in Si was by Zeindl *et al.*, (1987) who achieved δ doping using Sb, the favoured n-type dopant for Si MBE. The dopant profile was deduced from a combination of secondary ion mass spectroscopy (SIMS) and transmission electron microscopy (TEM) which suggested a layer width of ~ 2 nm.

Eisele (1989) reported the growth of Sb δ -layers in Si with a range of sheet densities from $\sim 10^{12}$ cm^{-2} to $> 5 \times 10^{14}$ cm^{-2} and, from TEM analysis, noted precipitates at doping levels $\sim 5 \times 10^{14}$ cm^{-2} . The degree of activation was investigated using Hall measurements carried out at 4.2 K to freeze out parallel conduction paths. A maximum sheet density $> 10^{14}$ cm^{-2} was obtained. The Hall mobility for the degenerate samples was almost independent of sheet density with a maximum value of ~ 100 cm^2/Vs . A more thorough investigation into Sb δ -layers was carried out by van Gorkum, Nakagawa and Shiraki, (1989).

Device applications for δ -layers in Si have also centred around FET structures. Zeindl, Bullemer and Temple, (1989) reported the fabrication of a MESFET with a degenerate conducting channel, the high-mobility heterojunction FET (Schubert *et al.*, 1987), light-emitting diodes (LEDs) (Schubert, Fisher and Ploog, 1985), and lasers (Schubert *et al.*, 1989).

The narrowest profiles display a full-width at half-maximum of only 2.9 nm (Schubert *et al.*, 1990a). Spatial localisation of dopants within a layer of thickness 1.5 nm was concluded from the SIMS measurements. The free-carrier mobilities were comparable to highly B-doped bulk Si. The growth, structural and electrical characterisation of Si:B delta structures were first reported by Matthey *et al.* (1990 a,b) and Powell *et al.*, (1991). Headrick *et al.*, (1991) reported on δ -doping with one full monolayer coverage of B and Si.

1.5 Structure of the thesis

In this work, the principal interest is in the thermoelectric properties of 2DHG and 2DEG structures in zero magnetic field ($B=0$). The thesis is structured as follows. The basic properties of 2D structures have been explained in this introductory chapter. Chapter 2 reviews the related scattering mechanism along with the diffusion and phonon-drag contributions to the thermopower S (when $B=0$) of a 2DHG/EG, when a temperature gradient is applied along the interface. The diffusion contribution is calculated by linearising and solving the Boltzmann equation in the relaxation time approximation. Moreover, an additional term that describes the carrier-phonon coupling is included for calculating the phonon-drag contribution.

In Chapter 3, two types cryostats are described for electrical characterisation of the samples: high temperature measurement cryostat and low temperature measurement cryomagnetic cryostat. Home-designed cryostat is

shown for thermal conductivity and thermopower measurements. Experimental procedure and sample design are also stated in this chapter.

Chapter 4 presents the experimental results of conductivity and Hall measurements for 2DHG SiGe heterostructure. Thermal conductivity, phonon mean free path and thermopower results for 2DHG and 2DEG structures are shown as experimental data and theoretical calculations are given for fitted thermopower data.

Chapter 5, the studies of the kinetic properties of Si single crystal with δ -<Sb> and δ - layers of various sheet densities furnish detailed information on the low temperature features of the carrier transport in these systems. Thermal conductivity and thermopower results are given in respect of both 2DEG and 2DHG systems. Theoretical calculations are carried out for many subband δ - 2DHG samples.

In Chapter 6, electrical and thermal measurements are summarised for 2DHG/EG Si/SiGe/Si (001) and Si- δ MBE grown samples. Further work is suggested for thermopower measurements are needed to make with magnetic field to see both the longitudinal and diffusion thermopower and transverse (Nernst-Ettinghausen) diffusion thermopower and the phonon drag contribution to the magnetothermopower.

CHAPTER TWO

REVIEW OF THEORY

AND

EXPERIMENTS

2.1 Introduction

In this chapter we present the theoretical background to the study of the semiclassical transport properties of a 2DHG and 2DEG. The transport coefficients are calculated by solving the Boltzmann equation in the relaxation time approximation. The concept of scattering mechanisms is introduced and the importance of screening in low dimensional transport calculations is presented. Particular emphasis is given to the thermoelectric coefficients associated with the thermoelectric currents produced when a weak thermal gradient ∇T is applied in the plane of the 2DHG. The diffusion and the phonon drag contributions to the thermoelectric coefficients are explained in both zero magnetic fields in this chapter. The literature on the thermopower of previous experimental and theoretical investigations is given in two dimensional systems.

2.2 Macroscopic transport equations

Let us consider a homogeneous, non-interacting 2DHG in thermal equilibrium in the absence of applied fields. The macroscopic transport equations in an isotropic conducting medium in the presence of an electric field $\mathbf{E}$ and a temperature gradient ∇T can be expressed as (Butcher, 1990 and Butcher, 1993):

$$\mathbf{E} = \rho \mathbf{J} + S \nabla T \quad (2-1)$$

$$\mathbf{Q} = \Pi \mathbf{J} - \lambda_L \nabla T \quad (2-2)$$

in the xy-plane, the 2D system is slightly perturbed from the equilibrium. As a response to this perturbation, the 2DHG produces macroscopic electric current, $\mathbf{J}$, and heat current, $\mathbf{Q}$, density. The scalar coefficients are electrical resistivity ρ , thermopower S , Peltier coefficient Π and lattice thermal conductivity λ_L .

Furthermore, by writing out the Boltzmann transport equation it is possible to derive an expression for the diffusion thermopower in the relaxation time approximation, for a distribution of electrons in a thermal gradient and combining these with system flux equations. However the route is simpler via the Peltier coefficient. In practice, S is measured by setting $\mathbf{J}$ to zero in Eq. (2-1) and measuring the temperature gradient and the resulting electric field.

2.3 Scattering mechanisms

In the following section, scattering mechanisms are considered in evaluating the thermopower of 2DHG (or 2DEG) in modulation doped SiGe

quantum well heterostructures. The thermopower depends strongly upon the various electron scattering mechanisms. If electrons/holes moving in the periodic potential were not scattered they would have an infinite electrical conductivity. Scattering can be divided into elastic and inelastic events.

Elastic collisions conserve both momentum and energy. In the 2D conducting channel for electrons, the dominant scattering process at low temperatures is impurity scattering. Ionised dopant atoms cause a Rutherford type scattering. In two dimensional systems, there are a number of scattering mechanisms such as interface roughness (Ando, 1977) and alloy disorder (Kearney and Horrell, 1998) in SiGe alloys. This surface roughness scattering can be particularly important in Si MOSFET devices. Scattering from neutral impurities is of little importance. The problem of elastic electron scattering by ionised impurities has been formulated by Stern and Howard, (1967).

Inelastic collisions are concerned largely with electron phonon interactions. Longitudinal acoustic (LA) phonons are the dominant scatters in lightly doped semiconductor crystals at low temperatures where the optical phonon occupation number is very small. Longitudinal acoustic phonons are like sound waves. The simplest coupling to electrons for phonons is through the deformation potential. The phonon compresses and dilates alternating regions of the crystal. A uniform compression or dilation of the crystal causes the edge of each electronic energy band to move up or down proportionally to the strain. The constant of proportionality is called the deformation potential (Davies, 1998). The effect on the charge carriers is described in terms of a deformation

potential or, at low temperatures for example in GaAs, piezoelectric effects. The deformation potential scattering is complicated in n -type Si by intervalley scattering. Once again a number of workers have provided theoretical treatments for the scattering of quasi-2D electrons from acoustic phonons.

An interesting aspect of the phonon drag thermopower in 2DEGs and Si/SiGe is the relative importance of the different scattering processes for electrons and phonons. Thermal conductivity is dominated by phonons and contrary to normal metals the electronic contribution is negligible. The process limiting the phonon mean free path l_p at low temperatures is scattering at the sample boundaries giving a constant l_p (Tieke, 1997).

Expressions for the thermopower in quasi-two dimensional semiconductor quantum well structures are obtained in the extreme quantum limit when electrons are scattered by acoustic phonons via deformation potential coupling and ionised impurities. The scattering due to the electron-phonon interaction is supposed to be weak. Nevertheless, it produces the phonon drag thermopower, S_g .

2.4 Screening in 2D carrier systems

A space charge of electron/hole has the effect of screening any potentials in the vicinity. The electrons rearrange themselves in order to maintain a constant electro-chemical potential which reduces its strength. Screening is usually considered as an increase in the dielectric constant, ϵ , of the material although it is unrelated to ϵ . The phonons cause local variations in the lattice

constant and thus the energy of the conduction band edge, which is described by a deformation potential. We assume that holes, which are confined in a quantum well, occupy only the ground subband in modulation doped Si/SiGe heterostructures.

A mathematical description of screening in the modulation doped case, where the 2DEG and 2DHG are heavily degenerate $(E_F - E_0) \gg k_B T$ at low temperatures is provided by Bastard (1988). The dielectric function is often written in the 2D Thomas-Fermi approximation as:

$$\varepsilon(q) = 1 + \frac{q_s}{q} \quad (2-3)$$

where q_s is the 2D screening constant:

$$q_s = \left(\frac{e^2}{2\varepsilon\varepsilon_r} \right) \frac{\partial n_s}{\partial E_F} = \frac{m^* e^2}{2\pi \varepsilon \varepsilon_r \hbar^2} \quad (2-4)$$

(Ando, Fowler and Stern; 1982) and q is the in plane component of wavevector. There is a cut off in scattering for $q > 2k_F$ which corresponds to the minimum length scale on which the electron charge density can vary.

For screening of phonons, in the Thomas Fermi approximation,

$$\Xi(q) = \left(1 + \frac{q_s}{q} \right)^{-1} \Xi \quad (2-5)$$

where Ξ is the unscreened deformation potential.

We can see calculations of screened and unscreened deformation potentials in phonon-drag thermopower as an example. With only the introduction of screening, Smith and Butcher (1989a) clearly improved the agreement between theory and experiment. **Figure 2.1** shows their results for the

phonon drag thermopower for the screened and unscreened case for a GaAs/AlGaAs heterojunction calculation against temperature. It is observed that there is difference in an order of magnitude between screened and unscreened deformation potential in phonon drag thermopower curves. These calculations have been done for Si/SiGe heterojunction and delta and <Sb> doped Si and a large difference is observed for our samples (see Chapter 4 and Chapter 5).

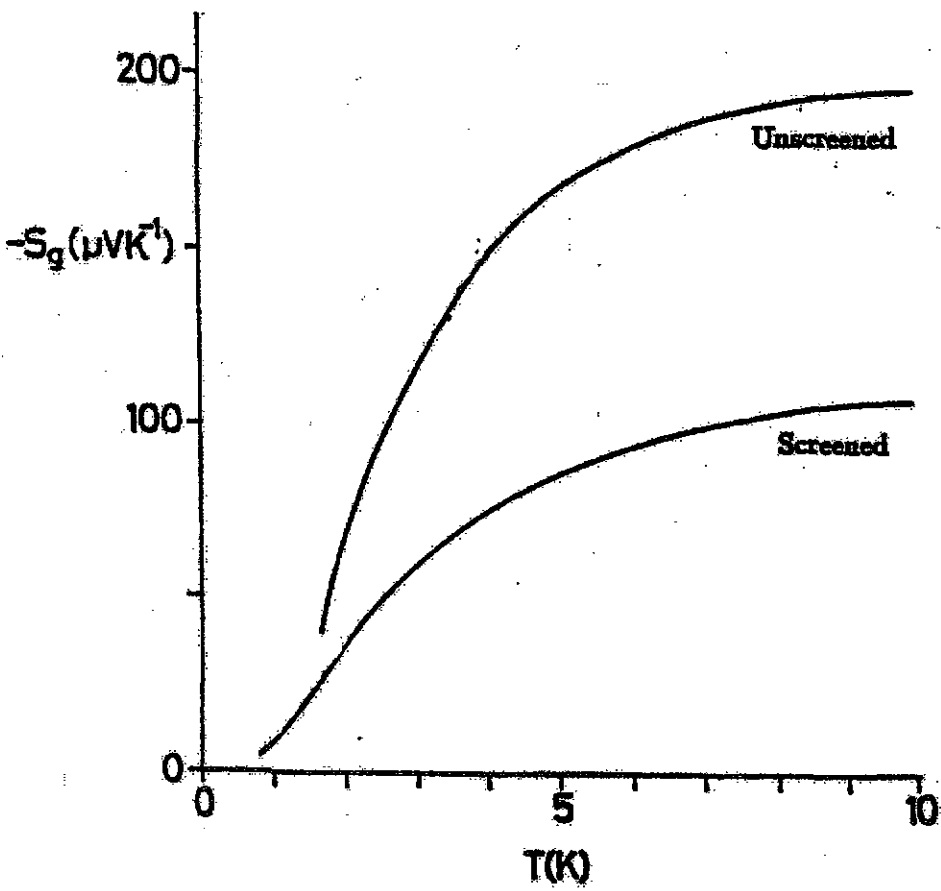


Figure 2.1: Calculations of S_g against T for $n_s = 1.78 \times 10^{11} \text{ cm}^{-2}$ in GaAs (After Syme, 1989).

2.5 Thermal conductivity

Heat transport in a solid is caused by phonons and all other mobile quasi-particles which contain excess energy and interact with the lattice, such as electrons and holes. The electronic components of heat conduction are usually the largest components in a metal, but almost all of the thermal current in a non-metal is carried by the lattice vibrations (phonons). It is necessary now to consider the magnitude of this phonon current when there is a finite temperature gradient.

In thermal equilibrium, if there is no temperature gradient the net heat flow will be zero. When a finite temperature gradient ∇T is established, the thermal conductivity λ_L can be defined in terms of ∇T and the rate of energy flow per unit area Q normal to the gradient (Kittel, 1967):

$$Q = -\lambda_L \nabla T \quad (2-6)$$

This thermal conductivity can be expressed in terms which relate to the microscopic properties of phonons by appealing to the analogy between conduction in a phonon 'gas' and in a conventional molecular gas. The thermal conductivity result of the kinetic theory of gases simplifies for the case of all particles having the same speed to (Ashcroft and Mermin, 1976)

$$\lambda_L = \frac{1}{3} C_v v_s l_p \quad (2-7)$$

Here C_v is the lattice specific heat per unit volume, v_s is the phonon velocity and l_p is the phonon mean free path. v_s :

$$\frac{1}{v_s^3} = \frac{1}{3} \left(\frac{1}{v_l^3} + \frac{2}{v_t^3} \right) \quad (2-8)$$

where v_s^{-3} is the average inverse cube of the speed of sound for the three acoustic modes. We note that, for the purposes of this analysis, the thermal conductivity of the entire strained layer (quantum well + substrate), may be used to deduce C_g in Eq. (2-16), since acoustic phonon modes (unlike the holes) experience no confinement in the Si-Ge alloy and v_t is acoustic transverse and v_l is longitudinal modes in (001) Si. The phonon specific heat C_v in the Debye approximation for the three acoustic branches is written in the form (Ashcroft and Mermin, 1976),

$$C_v = \frac{3}{2\pi^2} \left[\frac{k_B T}{\hbar v_s} \right]^3 k_B \int_0^{\theta_D/T} \frac{x^4 e^x}{(e^x - 1)^2} dx \quad (2-9)$$

where $x = \hbar v_s Q / k_B T$ and Q is the magnitude of the phonon wave vector. The influence of doping on the thermal conductivity of Si is illustrated in **Figure 2.2** (Boer, 1990).

2.6 Phonon mean free path

The critical parameter of the thermal conductivity is the mean free path, which requires a thorough study of the phonon scattering mechanisms. Boundary scattering is assumed to be the dominant process determining the phonon mean free path l_p . In SiGe/Si heterostructures, thermal conductivity is dominated caused by acoustic phonons in the bulk of the Si substrate at the low

temperatures, used in the experiments. At low temperatures ($T \leq 1$ K), defect, impurity and phonon-phonon scattering are negligible and l_p is limited by scattering at the sample boundaries, as first observed by Casimir (1938). The clean T^3 dependence observed in the experimental data is characteristic for a constant l_p in the boundary scattering limit since $C_v \propto T^3$.

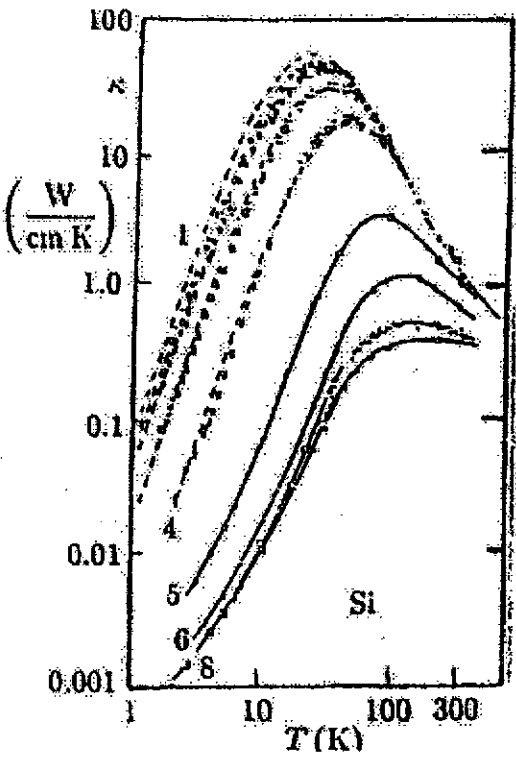


Figure 2.2: Influence of doping on the thermal conductivity for p-type Si with doping concentrations of 1×10^{13} , 4.2×10^{14} , 4×10^{15} and 4×10^{16} for curves 1-4 and for n-type Si with doping concentrations of 6.2×10^{19} , 1.7×10^{20} , 3×10^{20} and $3.5 \times 10^{20} \text{ cm}^{-3}$ for curves 5-8, (Taken from, Boer, 1990).

2.7 Thermopower

Thermopower can be defined as the ratio of the voltage difference to the temperature gradient. The thermopower (Seebeck coefficient) is given as (Syme, 1989):

$$S = \Delta V / \nabla T \quad (2-10)$$

where ΔV is the differential voltage increased as a response to a small temperature gradient ∇T .

In recent years there has been much interest in the properties of two dimensional electron and hole systems. The application of thermopower theory to 2DHGs has taken place only in the last fifteen years. In this thesis the thermoelectric phenomena in 2DHGs and 2DEGs has been carried out in zero magnetic field ($B=0$). This area can then be studied in terms of the diffusion and phonon drag contribution. The temperature gradient induces the motion of the charged carriers and the flow of phonons. The former yields the diffusion thermoelectric power S_d . The diffusion thermopower depends upon the energy dependence of the momentum relaxation times of the carriers. The latter imparts its momentum to the electron (or hole) system through electron-phonon interactions, creating another electronic current. This yields the phonon drag thermoelectric power S_g (Cantrell and Butcher, 1987a, Gallagher *et al.*, 1987 and Fletcher *et al.*, 1994). The phonon drag contribution to electrical conductivity is usually negligible (Blatt, 1968) but phonon drag plays a very important role in the thermopower. At liquid He⁴ temperatures phonon drag dominates the thermopower of single layer 2D systems.

The thermoelectric properties of conductors and semiconductors have been considered minor in comparison to other properties. However, in general, they are just as much bulk properties as, for example, the electrical or thermal conductivity of materials. Thermoelectric effects can be used to discover more about modern electronic materials. Indeed, various electrical parameters were discovered using the Seebeck coefficient.

Thermopower is useful in mapping the density of states and band structure of subbands in devices and of the mini bands formed in superlattice structures for similar reasons (Syme, 1989) and could be used for experimental determination of the deformation potential value as the fitting parameter in comparison experiments with the theory of phonon-drag thermopower.

2.7.1 Diffusion thermopower

The diffusion thermopower in the metallic regime is relatively well understood. This gives essential information on electron scattering, as well as a unique contribution, which arises from the dependence of S on the energy derivative of the scattering time τ .

The temperature gradient ∇T causes a diffusion of charge carriers, which results in a charge separation producing an electric field. The charge flow stops once the electromotive force balances the thermal force. As a result, there is a contribution to the thermopower, due to the diffusion of charges, called the diffusion thermopower.

The 2D current density response to an applied electric field $\mathbf{E}$ and temperature gradient ∇T takes the form:

$$\mathbf{J} = \sigma \mathbf{E} + L \nabla T \quad (2-11)$$

$$L = \frac{\pi^2}{3e} k_B^2 T \frac{d\sigma(E_F)}{dE} \quad (2-12)$$

Here, the conductivity σ and the coefficient L are both scalars. They are easily evaluated in the diffusive regime using either the electron Boltzmann equation or Kubo formulae. The Seebeck coefficient in the diffusion regime, S_d , is the ratio of $\mathbf{E}$ to ∇T when $\mathbf{J}=0$. So that,

$$S_d = L / \sigma = - \left(\pi^2 k_B^2 T / 3e \right) \left(d \ln \sigma(E) / dE \right)_{E_F} \quad (2-13)$$

here, E_F is Fermi level and $\sigma(E) = n_s(E) e^2 \tau(E) / m^*$ is the conductivity at absolute zero when the Fermi level is at E ($n_s(E)$ denotes the corresponding 2D electron density). For most energies and most scattering mechanisms $\sigma(E)$ increases with E . Eq. (2-13) then shows that S_d has the negative value which is commonly observed for electrons. However, when an electron moves into a new subband in a 2DEG there is a sudden increase in the density of final states available for scattering. Consequently, $\tau(E)$ shows a sharp decrease and so does $\sigma(E)$. When broadening effects are ignored, Eq. (2-13) predicts that S_d will exhibit a positive δ -function like peak when E_F enters a new subband (Wu, Horing and Cui, 1996). In reality, the peaks are broadened both thermally and by electron scattering (Cantrell and Butcher, 1985). The effect has been observed by Ruf *et al.* (1989).

The knee expected in σ when the second subband begins to populate has also been observed recently by Fletcher, Harris and Foxon, (1991).

The diffusion contribution S_d for a 2DHG in the degenerate limit shows linear temperature dependence via the Mott formula (Gallagher and Butcher, 1992):

$$S_d = (p+1) \frac{\pi^2 k_B^2 T}{3|e|E_F} \quad (2-14)$$

here, E_F is the Fermi energy. The parameter p ($p = (\partial \ln \tau / \partial \ln E)|_{E_F}$) is determined by the energy dependence of the transport lifetime τ . The parameter p is a function of sheet carrier density, n_s (calculated by Karavolas *et al.*, (1990)). It has been observed experimentally that $S_d \sim T$ (diffusion thermopower only) could be observed at $T < 1$ K and at $T > 60$ K for the highest sheet carrier density $n_s > 10^{12} \text{ cm}^{-2}$ for delta-doped GaAs quantum-wells (Fletcher *et al.*, 1994).

2.7.2 Phonon drag thermopower

The theory of the phonon-drag thermopower, S_g , of 2D electrons (or holes) coupled to 3D acoustic phonons in zero magnetic field has been formulated by Cantrell and Butcher (1987a). They derived an explicit formula for S_g by solving the coupled Boltzmann equations for the carriers (electrons or holes) and the phonons. The Cantrell-Butcher formula for S_g , has recently been refined to account for screening and the departure from full degeneracy,

(Ziannia, Butcher and Kearney, 1994, Fletcher *et al.*, 1994 and 1997, Butcher and Tsaousidou, 1998 and Tsaousidou *et al.*, 2000). This is given by,

$$S^g = \frac{(2m^*)^{3/2} l_p}{16\pi^3 \hbar k_B T^2 p_s |e| \rho} \sum_m \int_0^\infty \int_{-\infty}^\infty dq \, dq_z \, q^2 \, Q \frac{\Xi^2(\mathbf{Q})}{\epsilon^2(q)} N^0(\mathbf{Q}) \Delta(q_z) \times \int_0^\infty du \, f^0(u^2 + \gamma) [1 - f^0(u^2 + \gamma + \hbar\omega_Q)] \quad (2-15)$$

where m^* is the in-plane hole effective mass, l_p is the phonon mean free path, $|e|$ is the magnitude of the electronic charge, and ρ is the mass density. Moreover, ω_Q is the frequency of the phonon with wave vector $\mathbf{Q} = (\mathbf{q}, q_z)$ and mode m ($\mathbf{q}$ is the component in the plane of the 2DHG and q_z is the perpendicular component), $N^0(\mathbf{Q})$ is the Bose-Einstein distribution function for phonons in equilibrium, $\Delta(q_z)$ is a form factor that accounts for the finite thickness of the 2DHG, and $\epsilon(q)$ is static dielectric screening function (Ando, Fowler and Stern, 1982) (Full expressions for $\Delta(q_z)$ and $\epsilon(q)$ are given in Fletcher *et al.*, (1997)). The hole-phonon coupling is described by the ‘effective’ acoustic deformation potential $\Xi_{\text{eff}}(\mathbf{Q})$. For an anisotropic hole energy spectrum, both the longitudinal and the transverse acoustic modes couple to holes due to dilation and shear strain respectively. Here, we simplify our analysis by assuming that the hole density p_s is small enough so that we can treat the heavy hole subband as isotropic. In this case, the holes interact only with the longitudinal acoustic branch and the hole-phonon coupling is described by a single deformation potential constant. We determine the value of Ξ_{eff} by comparing the data with the theoretical estimates of S_g . It should be stressed that the value of Ξ_{eff} is the only

adjustable parameter in our calculations. Finally, in equation (2-15), f^0 is the Fermi-Dirac function which describes the hole distribution and $u^2 + \gamma$ is the hole energy E . The expression for γ is $\gamma = (\hbar\alpha_Q - E_q)^2 / 4E_q$ where $E_q = \hbar^2 q^2 / 2m^*$. Also

$$C_g = \frac{|e| \ell_p \Xi_{\text{eff}}^2 g_v (2m_{\parallel}^*)^{1/2}}{32\pi^3 \hbar k_B T^2 \rho} \quad (2-16)$$

where $m_{\parallel}^*$ is the carrier effective mass in the interface plane, ρ is the mass-density of the bulk material, g_v is the valley degeneracy, ℓ_p is the phonon mean free path and Ξ_{eff} is the effective acoustic deformation potential. For a spherical energy band Ξ_{eff} is a constant. In cases where the energy bands are not isotropic or the materials are piezoelectric, Ξ_{eff} requires modification.

Above 1 K phonons and electron-phonon interactions become increasingly important. We concentrate here on the thermopower of a 2D-EG/HG in the temperature range 1 to 25 K, which has been the subject of several recent experimental and theoretical investigations. To distinguish between diffusion and phonon drag thermopower, its temperature dependence is a suitable criterion. The diffusion thermopower is linear in temperature whereas phonon drag varies with a stronger power of temperature depending on the electron-phonon scattering mechanism involved.

2.7.3 Piezo-electric contribution to thermopower

In non-centrosymmetric crystals, a stress can induce a macroscopic electric polarisation field $\mathbf{E}$ in the crystal. This phenomenon is known as the

piezoelectric effect. This phenomenon can also be described as a strain inducing an electric field (Yu and Cardona, 1996).

The two contributions, longitudinal acoustic (LA) and transverse acoustic (TA) phonons to the piezoelectric electron-phonon scattering are included in the following expression

$$\Xi_{\text{eff}}^2(Q_l) = \Xi_d^2 + (eh_{14})^2 \frac{A_l}{Q^2} \quad (2-17)$$

and

$$\Xi_{\text{eff}}^2(Q_t) = (eh_{14})^2 \frac{A_t}{Q^2} \quad (2-18)$$

here h_{14} is the piezoelectric constant and A_l , A_t are anisotropy factors. In a cylindrically symmetrical system (Ridley, (1988), Smith and Butcher, (1989a) and Zianni, Butcher and Kearney, (1994))

$$A_l = \frac{9q^4 q_z^2}{2Q^6} \quad (2-19)$$

$$A_t = \frac{8q^2 q_z^4 + q^6}{2Q^6} \quad (2-20)$$

when the conduction band is anisotropic, like Si, both LA and TA phonons interact with electrons via the deformation potential Ξ_u .

When an electric field is applied to a piezoelectric material, it strains due to the converse piezoelectric effect. Exact correspondence with the experiment is obtained only if scattering of the acoustic mode phonons by both the deformation potential and the piezoelectric coupling mechanisms are considered. Xie *et al.* (1986) deduced a value for the piezoelectric constant for $\text{Si}_{0.8}\text{Ge}_{0.2}$.

Khizny *et al.* (1996) reported the first direct experimental evidence for the reversible wave to sound wave conversion of a high frequency electric field within a MBE grown SiGe/ (001) Si strained layer sample. On the other hand, they could see no such effect for either Si:B δ -doped homojunction samples or standard Si substrate samples. Contribution of piezoelectric to the thermopower has been carried out theoretically and compared with experimental data for SiGe/Si heterostructures samples used in this work (see Chapter 4).

2.8 The Kohn anomaly in thermopower

The temperature dependence of S_g is principally determined by the need to conserve momentum in the plane of the two-dimensional carriers. Maximum momentum transfer leads to an enhancement of phonon-drag thermopower. The condition for maximum momentum transfer yields to the ‘Kohn anomaly’ and should occur for $q_D = 2k_F$, where $q_D = 5k_B T / \hbar v_s$ is the dominant phonon wavevector with v_s sound velocity, and $k_F = (2\pi n_s / g_v)^{0.5}$ is the Fermi wavevector of carriers (valley degeneracy $g_v = 1$ for p-type and $g_v = 2$ for n-type (100) Si samples). This ‘Kohn anomaly’ is much stronger in 2D than in 3D because of the restriction in phase space, but the averaging over transverse and longitudinal modes of phonon velocities broadens it. Experimentally, the Kohn anomaly has been reported for various 2D single subband occupied systems (Gallagher and Butcher, 1992). When the temperature dependence of the ratio S/λ_L is analysed, the expected position T^{KA} of the resonance $q_D = 2k_F$ is given by:

$$T^{KA} = 2(\hbar v_g / 5k_B)(2\pi n_g / g_v)^{0.5} \quad (2-21)$$

2.9 The thermopower literature

The thermopower for a free-electron gas, as calculated from the Boltzmann equation, should be linear in temperature, and involves a contribution from the derivative of the scattering time with respect to energy evaluated at the Fermi energy (Ridley, 1982 a). Electron - phonon scattering is theoretically predicted in GaAs / Ga_{1-x}Al_xAs type structures (Lee, Spector and Arora, 1983). For impurity scattering the scattering time is sensitive to the scatterer (remote or background), the wave functions of the electrons and the strength of the screening by the 2DEG. For conditions of strong screening and background impurities, this calculation also finds the energy dependence of the scattering time to be independent of energy. Since our determination of the thermal gradient limits the ability to definitely state that the scattering is independent of energy, it is at least consistent with calculations of the scattering time. In this situation the expression for the thermopower by Davidson *et al.*, (1986),

$$S = \frac{4\pi^3 m^* k_B^2 T}{3eh^2 n_s} \quad (2-22)$$

This expression is valid for an ideal 2DEG as long as the temperature is well below the Fermi temperature.

Thermopower data gives valuable information about electron (or hole) transport processes in metals and semiconductors. A lot of work exists in the literature on thermopower in heterostructures (Karavolas *et al.*, 1990, Zianni, Butcher and Kearney, 1994 and Fletcher, Pudalov and Cao, 1998) but little published data about Si /SiGe modulation doped two dimensional systems (Mironov *et al.*, 1997).

In a Si-MOSFET, electrons are assumed to interact with phonons via a deformation potential. Because of elastic anisotropy the situation is very complicated. It is necessary to consider each direction of the phonon wave vector $\mathbf{Q}$ separately in calculating the transition rate as it has been done by Herring and Vogt, (1956). However, it is possible to use a simpler approach that involves an implicit averaging over the azimuthal angle of $\mathbf{Q}$ and regarding elastic anisotropy as small. Accounting for both the longitudinal (LA) and the transverse (TA) acoustic phonons the square of the matrix element is taken as Ref. (Ridley, 1982b) and some details are given in Ref. (Zianni, 1993).

III-V heterostructures were studied by Nicholas *et al.*, (1985). They reported that the thermopower of GaInAs-InP heterojunctions varied approximately as T^{-1} at low temperatures (below 10 K) and then as T^n above 40 K, with $2 < n < 4$ depending upon the sample. Vuong (1985) found that the thermopower of GaInAs-AlInAs heterojunctions also varies as T^{-1} at low temperatures while GaAs-AlGaAs heterojunctions and superlattices have a roughly constant thermopower at low temperatures. Obloh, Klitzing and Ploog, (1984) have also measured the thermopower of GaAs-AlGaAs heterojunctions in

the range $1.5 \text{ K} < T < 50 \text{ K}$. Zavaritsky and Zavaritsky (1982) studied hole gases in germanium. They found the thermopower varied as T^n with $3 < n < 4$ over the range $2 < T < 20 \text{ K}$.

Lei (1994) and Xing *et al.*, (1995) have obtained S_d as the diffusion component. When there is no current flow in the y direction, it matches the result obtained from the Boltzmann equation with a constant relaxation time assumption in Ref. (Hicks and Dresselhaus, 1993).

The thermopower for the two channel conduction (parallel conduction) is

$$S = \frac{\sigma_n S_n + \sigma_p S_p}{\sigma_n + \sigma_p} \quad (2-23)$$

where $\sigma_{n,p}$ and $S_{n,p}$ are, respectively, the conductivities and the thermopower corresponding to electrons and holes (Zvyagin, 1991).

A formula for the phonon drag contribution, S_g , to the thermopower has been derived in (Cantrell and Butcher, 1987a, b), in which the coupled electron and phonon Boltzmann equations are linearized and solved in the relaxation time approximation at low temperatures where only acoustic phonons are important. Lyo (1988) follows the same way and points out that the contribution of piezoelectric scattering to S_g is about the same as that of deformation potential scattering in GaAs/AlGaAs heterojunctions.

Okuyama and Tokuda give,

$$S_g = S_g^{\text{DP}} + S_g^{\text{PE-L}} + S_g^{\text{PE-T}} \quad (2-24)$$

Here DP, PE-L and PE-T are deformation potential, piezoelectric-longitudinal and piezoelectric-transverse contributions to the phonon drag thermopower, respectively. All details are discussed in Ref. (Okuyama and Tokuda, 1990).

Another simple way to derive approximate formulae for S_g which are appropriate in various limits, has been reviewed by Smith and Butcher (1989 a, b).

$$S_g = -\frac{\alpha L_z C_v}{3n_s e} \quad (2-25)$$

here α is the fraction of the phonon momentum annihilated each second which appears in the electron system; L_z is specimen thickness, C_v is the phonon specific heat and n_s is carrier sheet density.

The expression for S_g in 2D becomes (Oxley, 1991):

$$S_g = -\frac{C_v L_z}{3n_s e} \frac{l_p}{v_s \tau_{pe}} \quad (2-26)$$

Hence $S_g \propto l_p T^3 / n_s$ at low temperatures. τ_{pe} is independent of n_s but determines the phonon momentum transfer rate to electrons. Although it is only weakly temperature dependent, and enhancement of S_g is expected if the dominant phonon wavevector coincides with $2k_F$.

Zavaritsky and Kvon (1983) used the theory outlined in Zavaritsky and Zavaritsky (1982) to obtain a value of 8 eV for the deformation potential of silicon. Zavaritsky and Kvon also investigated the ratio of thermopower to thermal conductivity, S/λ_L . This is expected to give a measure of the electron-phonon interaction. They found a peak at a temperature T^d that varied with

carrier density n_s . This corresponds to $q=2k_F$ for the Kohn anomaly, and reasonable numerical agreement was obtained.

Zavaritsky (1984) found an expression for S_g/λ_L for the case of $q_{||}>1$ and $q_{||}<<k_F$, which when altered to be dimensionally correct is

$$S_g / \lambda_L = - \frac{m^{*2} \Xi^2}{3\pi |e| \hbar^3 n k_F \langle v \rangle^2 a \rho} \quad (2-27)$$

here ρ is the (mass) density of the sample and Ξ is a deformation potential constant. This predicts S_g/λ_L to be of order 1 $\mu V.m/W$ for a (100) Si inversion layer. For typical values of n and a this is the correct order of magnitude. He also claimed to have observed the m^{*2} dependence by comparing S_g/λ_L for (100) and (111) electron inversion layers and (111) hole inversion layers, but there was no the evidence for this.

More accurate expression for the phonon drag contribution (arises from the phonon momentum transfer to the 2D holes through the hole-phonon interaction (Smith, 1979) is given by (Zianni, Butcher and Kearney, 1994). Extensive calculations of S_g have been made by Smith and Butcher (1989a, b), Gallagher *et al.* (1990) and Lyo (1988) for Si MOSFET and GaAs/AlGaAs heterojunctions. All the parameters needed are measured in other experiments and are known in principle. But, there is considerable uncertainty in some of their values. They compare values of $-S_g/T^3$ calculated for a Si MOSFET with measured values of the total thermopower divided by $-T^3$ (Gallagher, *et al.*, 1990). The data points are fairly flat for $T > 2.5$ K, which reflects the basic T^3 dependence predicted by the elementary treatment. The measured values also

increase as n_s decreases in rough accord with the n_s^{-1} behaviour predicted there. What is not predicted by the elementary treatment is the maximum exhibited by the data at a temperature proportional to $n_s^{-1/2}$. This behaviour is due to “Kohn anomaly”.

Fletcher *et al.* (1997) gives an expression for phonon drag thermopower, which is $S_g \propto T^6$. In this limit $S_g \propto n_s^{-3/2}$ via the factor k_F^{-3} , the result is independent of m^* and the details of the electronic wave function. With piezoelectric coupling, which is appropriate in GaAs, the magnitude remains much larger owing to the lower temperature.

CHAPTER THREE

EXPERIMENTAL

3.1 Introduction

The measurements presented in this thesis are of three types - electrical, thermal and thermoelectric. Each measurement has been done under specific experimental conditions. The requirements for the thermoelectric measurements are split into the thermal and electric parts. The following sections describe cryostats that allowed the electrical, thermal conductivity and thermoelectric power of the devices investigated to be measured to considerable accuracy.

3.2 Molecular Beam Epitaxial Growth

The Solid Source Molecular Beam Epitaxy (SS-MBE) technique is used for the growth of high-quality quantum wells. MBE has made a great impact on semiconductor physics and technology. MBE growth of SiGe/Si heterostructures and delta boron (B) and antimony (Sb) doped structures discussed in this study

was performed using a VG V90s built by Vacuum Generators Ltd. in Maunsell UK. A detailed description of the Si MBE system design and operation is given by Kubiak, Parker and Lye, (1988) and **Figure 3.1** shows a schematic diagram of the growth chamber.

Typically, base pressures of 10^{-11} mbar ultra high vacuum (UHV) conditions were achieved thus reducing unwanted impurity adsorption from the residual gas. To improve the vacuum conditions, the chamber was cleaned, often with water and with liquid nitrogen. The cleaned 4-inch substrate was placed in a vacuum chamber. The substrate was made to rotate during growth to ensure a uniform temperature and uniform distribution of alloy and dopant across the entire wafer. Si and Ge deposition/ co-deposition was made using separate electron beam evaporators (e-guns) from solid source charges. Shutters were placed above these sources to screen them from the wafer allowing the beams to be terminated instantaneously by opening or closing the relevant shutter. SiGe heteroepitaxial and delta and <Sb> doped Si layers were deposited on clean Si (001) substrates. MBE offers the unique advantage, perhaps, of allowing the crystal growth to produce a dopant sheet in the semiconductor which is confined to a region of one or two atomic layers and which is therefore only a few angstroms in thickness (Powell *et al.*, 1991). Growth occurs two-dimensionally offering the prospect of a monolayer resolution of the doping profile.

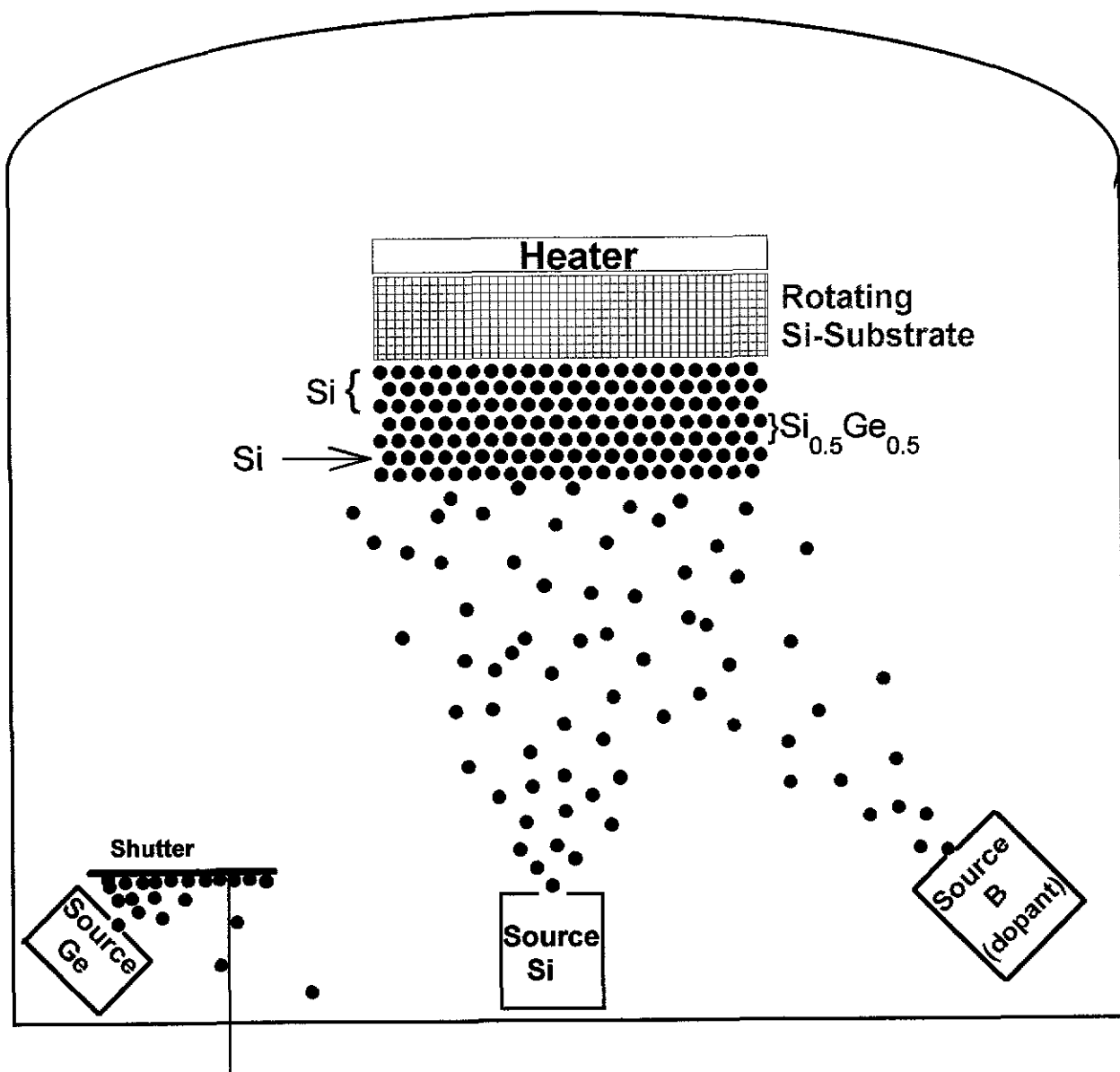


Figure 3.1: Schematic of the Si-Molecular Beam Epitaxy (MBE) Growth System.

3.3 Hall effect measurement systems

In this section the cryogenic system and experimental van der Pauw method for electrical measurements, including resistivity and Hall effect measurements are explained. The methods of achieving the electrical measurements are provided including device production, measurement system and cryostat facilities.

3.3.1 Sample preparation

Epitaxial samples of the required van der Pauw geometry were obtained by cleaving a square with an approximate side length of 6 mm from the wafer. Although this shape is suitable for the resistivity and low field Hall measurements, mesa etched Greek cross geometry is preferred. Specimens must have uniform thickness, which is not a problem for epitaxial material. The first stage in the fabrication process was to deposit 1 mm diameter discs of aluminium (Al) (1% Si) on the corners which was done using an ION TECH LTD (Microvac 350) magnetron Sputterer. The samples were then annealed in N₂ gas at 470- 520 °C for 40-80 min, in order to diffuse Al from the surface to the 2DHG in sufficient quantity for ohmic contact formation. Ohmic contacts were prepared by the sputtering of Al dots through a shadow mask, to a thickness of 0.5 µm. The annealing temperature and duration depends on cap layer thickness.

The van der Pauw geometry was defined by painting a black wax cross, so as to connect four Al ohmic pads. Etching of the wafer for 10s in CP4A, a

mixture of HNO_3 , CH_3COOH and HF acids in the ratio 75:17:8 followed by cleaning in xylene to dissolve and remove the wax, left the 2DHG in a mesa cross structure, about 10 μm in height, ready for electrical assessment. The technique is particularly useful in that no lithographic stages are necessary.

3.3.2 Measurement apparatus (1.6-300 K)

The cryostat design has been developed and refined by the I.L.L. for resistivity and Hall effect measurements in the 1.6-300 K temperature range. A schematic diagram of this cryostat is shown in **Figure 3.2**. Complete separation between the variable temperature insert and the helium container by the liquid nitrogen shield allows samples to be heated to 300 K with no increase in the consumption of liquid helium. Separation between the cooling system and the sample considerably reduces the risk of blockage in the cooling system. After reaching a temperature of 4.2 K the lowest temperature of 1.6 K was achieved by pumping the liquid helium around the sample chamber. A cold valve design (V3), which can be opened for rapid cooling and when closed maintains a flow, eliminates regulation problems. All separate volumes are fitted with pressure relief valves with the exception of the liquid nitrogen container that is opened to the atmosphere. A carefully designed sample holder is provided on which samples can be mounted in close contact with a Si diode thermometer, calibrated in the range 1.5-300 K with an uncertainty of ± 30 mK. The baffles on this sample holder ensure correct thermal coupling between the sample holder and the cooling gas. Hall effect measurements were performed in a magnetic field of

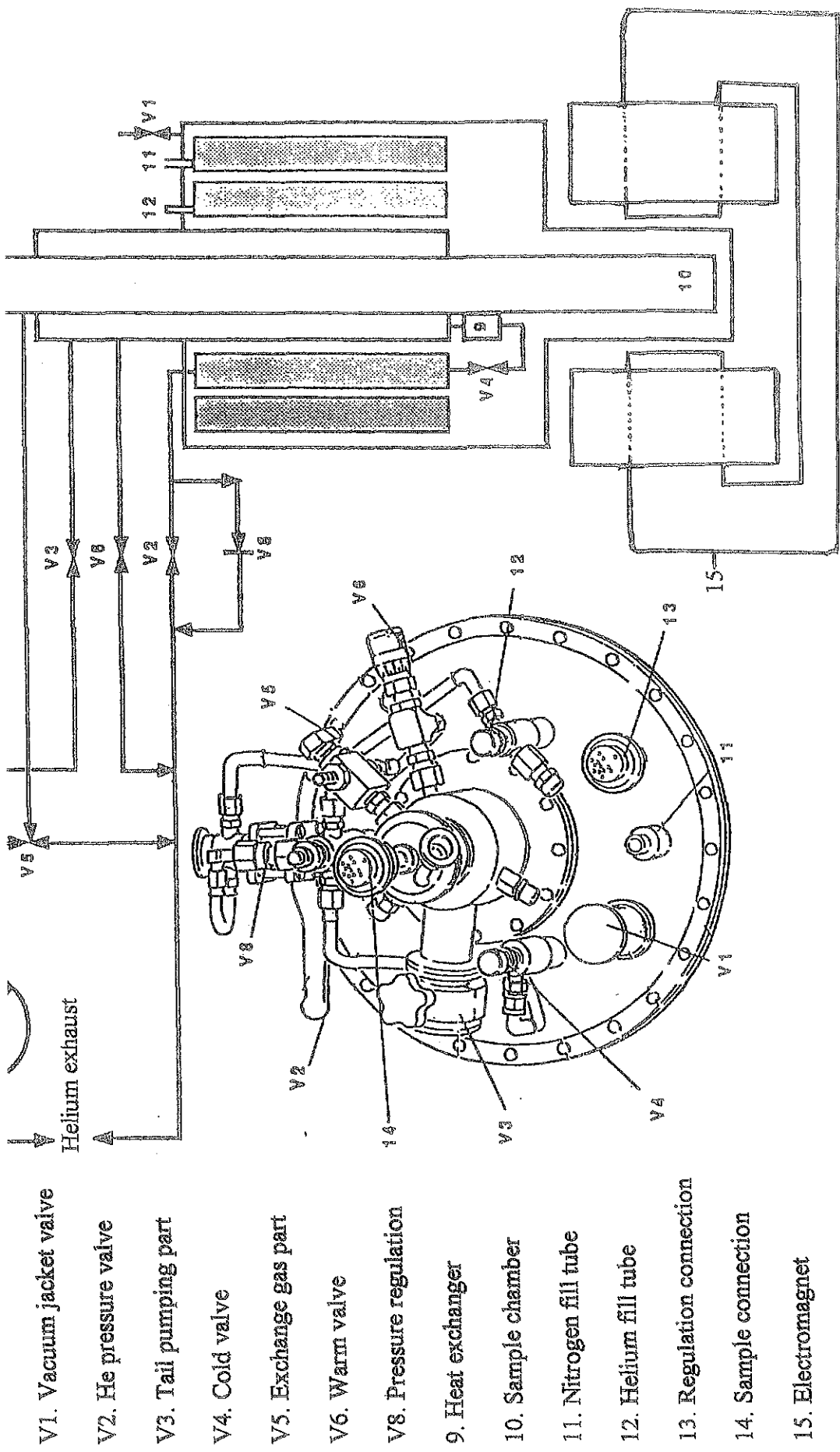


Figure 3.2: Schematic diagram of the ILL "Orange" cryostat used for electrical measurements

(After Sadeghzadeh, 1998).

maximum 0.65 T obtained by a water-cooled electromagnet with its jaws adjusted so as to accommodate the tail of the cryostat enabling the sample to be positioned at the centre of the pole piece region.

3.3.3 High temperatures transport measurements

The low field Hall coefficient and resistivity were measured simultaneously for temperatures from 1.6 K to room temperature using the I.L.L. “Orange” cryostat. Easy and fast to process, the van der Pauw device was used for the basic characterisation needs. Two common geometries for the van der Pauw method of measuring the Hall coefficient and resistivity in a thin sample are shown in **Figure 3.3**. This method is particularly convenient for a disc of irregular shape. These measurements were made using an EG&G Princeton Applied Research (Model 5208) lock-in amplifier as both ac signal (0-5V) source and voltage detector. The current used was kept as low as possible, well within the ohmic region to avoid hot-electron effects, e.g. the maximum voltage applied across samples of 6 mm length was kept below 10 mV at low temperatures.

The resistivity (at $B=0$) was measured at the same current as the Hall effect by the 4-contact method (van der Pauw 1958) as:

$$\rho = \frac{\pi t}{\ln 2} \frac{V_{AB,CD} + V_{BC,DA} + V_{CD,AB} + V_{DA,BC}}{4I} f \quad (3-1)$$

where t is thickness of the sample which is taken as unity in two-dimensional cases, and $V_{AB,CD}$ for example is the measured voltage between contacts A&B while the current was passing through contacts C&D. The dimensionless

parameter f depends on the ratio of the measured voltages of different configurations.

The current is fed through the opposite contacts B&D and A&C while the Hall voltage is measured remaining the contacts A&C and B&D (**Figure 3.3.b**). Applying a perpendicular magnetic field B to the specimen face, van der Pauw showed that the Hall coefficient is given by:

$$R_H = \frac{\bar{V}_H}{IB} \quad (3-2)$$

where $\bar{V}_H$ is the average of the Hall voltages for different configurations and field directions. For the Hall effect, the magnetic field strength was 0.41 T. The small magnetoresistance component was eliminated by reversing the direction of the magnetic field for each measurement and taking the average of the magnitude of the Hall voltage for the two field directions. The factor R_H is called the Hall factor. Its magnitude depends on the scattering mechanisms that contribute to τ and is usually of the order of unity (McGregor *et al.*, 1999). Finally the two-dimensional hole sheet density is obtained by:

$$n_s = \frac{1}{eR_H} \quad (3-3)$$

Eq. (3-3) shows the relationship between sheet concentration, n_s and the sheet Hall coefficient R_H . In principle we can determine the carrier mobility by measuring R_H and ρ to obtain the Hall mobility is given by:

$$\mu_H = \frac{R_H}{\rho} \quad (3-4)$$

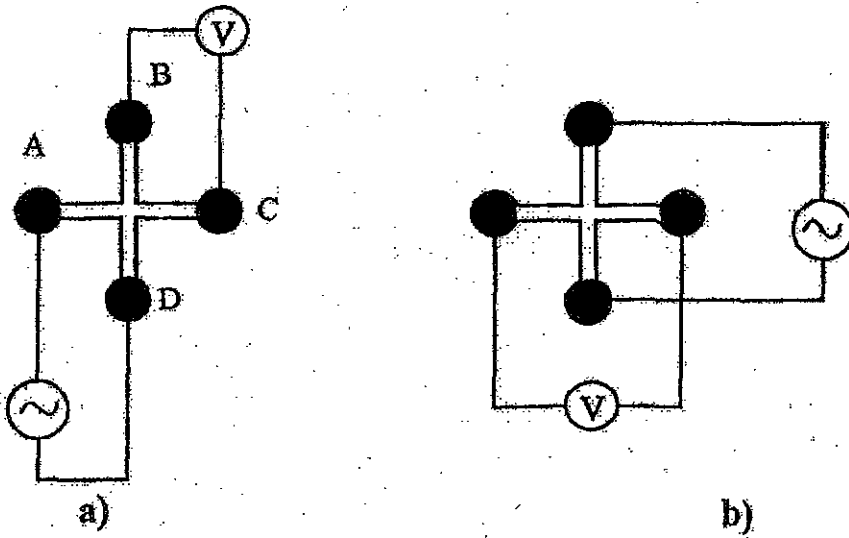


Figure 3.3: a) Resistivity and b) Hall measurement circuit of a Van der Pauw Greek cross shape device.

3.4 Cryomagnetic system (0.3 K)

Low temperature measurements have been carried out using cryomagnetic cryostat to measure the dependence of resistivity on temperature and Shubnikov de Haas oscillations described in following sections.

3.4.1 Hall bar devices

For the low temperature and high field magnetoresistance (MR) measurements, a well-defined rectangular geometry is needed for a much more detailed study of the 2DHG properties. Hall bar mesa structures were fabricated for the author using resists, photolithography and etchings. Specimens were then checked to ensure that the contacts were Ohmic and that all equivalent pairs of

contacts had similar resistances. The 2.25 mm×4.5 mm Hall bar chips were cut by a fine diamond saw and glued into a gold plated ceramic package (Epak Electronics). Typical Hall bars have a 3200 μm and 320 μm channel length (L) and width (w) respectively, with a 1600 μm voltage probes separation (ℓ). The bond arms of the package are gold wires bonded to the aluminium contact pads of the Hall bar.

3.4.2 Low temperature measurement cryostat

Low temperature measurements of resistivity and magnetotransport were carried out using an Oxford Instruments cryomagnetic system fitted with a base temperature of 0.33 K and a superconducting solenoid vertical magnetic field of up to 12 T. A schematic diagram of this cryostat is shown in **Figure 3.4**. The end of this part, which contains the sample and temperature sensors, is located in the centre part of a liquid ^4He bath. In order to obtain the lowest possible temperatures (0.33-1.5 K), first the 1 K pot, with temperature sensing performed by a capacitor connected to the 'LakeShore' controller was filled by ^4He and pumped continuously to give a base temperature about 1.4 K. Then ^3He was condensed inside the sample space and pumped on using a charcoal sorb. A top loading probe enabled the sample to be lowered directly into the insert, without losing the ^3He . The sorb (and hence sample) temperature was controlled automatically by an Oxford Instruments ITC4 controller.

A doped Ge resistance thermometer (Lake Shore Cryotronics) calibrated in the range 0.3-4 K and a Si diode between 4 K and 300 K were used for

measuring the temperature when in a stable condition and in the absence of a magnetic field. In Shubnikov-de Haas experiments the temperature measurements were taken at the start and finish of the run to check the stability and average. The magnetic field was provided by passing a direct current through the superconducting coil. The magnetic field which depends linearly upon the current can be varied continuously and reaches 12 T with 100 A.

3.4.3 0.3 K, 12 T Hall measurements

The longitudinal ρ_{xx} and transversal ρ_{xy} resistivities of 2DHG were measured on Hall bar geometry samples using the Oxford Instrument Cryogenic system down to 0.33 K. The Hall bar sample is shown in **Figure 4.19(b-2)**. In order to avoid carrier heating, a small (20 nA) ac (7 Hz) is passed through the sample, 10 k Ω and 47 M Ω resistors. By measuring the voltage V_{xx} , the longitudinal resistivity can be determined by:

$$\rho_{xx} = \frac{V_{xx}}{I} \frac{w}{\ell} \quad (3-5)$$

where w is the channel width and ℓ is the separation of the voltage probes.

The transverse resistivity ρ_{xy} is obtained by measuring the Hall voltage V_{xy} in the presence of a magnetic field similar to the Van der Pauw case. The lock-in amplifiers (EG&G Princeton Applied Research Model 5209) were used for increasing the current (via the voltage across the 10 k Ω resistor), V_{xx} and V_{xy} . The use of a lock-in amplifier increases the ultimate sensitivity for measurement of Hall voltages on low resistance samples. Low temperature

magnetotransport was performed at a constant temperature while the magnetic field was swept continuously up to 12 T by measuring the current through the superconducting coil at a rate of 1 A/min (1T = 8.36 A). The system was computer controlled and the data were stored in a computer for subsequent analysis.

3.4.4 Shubnikov-de Haas oscillations of magnetoresistance

Magnetic fields at which ρ_{xx} and σ_{xx} have minima correspond to an integral number of filled Landau levels, since the Fermi level is midway in between the extended state regions: in these cases, the system behaves as an insulator. On the other hand, when the highest occupied Landau level is only half full, then by definition the Fermi level is at the centre of a region of de-localised states, and so the sample look like a metal. Consequently the conductivity, σ_{xx} , has a maximum and the reason why the resistance, ρ_{xx} , simultaneously has a maximum is that there are many vacant states next to the Fermi level for scattering holes into. So as the magnetic field is increased, the resistivity oscillates from large to small and back again. This is called Shubnikov-de Haas oscillation and is shown in **Figure 3.5**.

At small B the oscillations are caused by the spin-up Landau level overlapping with the spin-down Landau level adjacent to it. As the magnetic field is increased these two levels separate. As the temperature is increased the smearing of the Fermi surface means that the Landau quantisation has no effect on transport properties.

The small signal oscillations are described by the equation (Coleridge *et al.*, 1989)

$$\frac{\Delta\rho_{xx}}{\rho_0} = R_s V \frac{\xi}{\sinh \xi} \exp\left(\frac{-\pi}{\omega_c \tau_q}\right) \cos\left(2\pi \frac{E_F}{\hbar\omega_c} + \phi\right) \quad (3-6)$$

where R_s and V are constants related to spin reduction factor (Schoenberg, 1984) and scattering mechanisms,

$$\xi = \frac{2\pi^2 kT}{\hbar\omega_c} \quad \text{and} \quad \omega_c = \frac{eB}{m^*} \quad (3-7)$$

The amplitude of the oscillations is defined as:

$$E = R_s V \frac{\xi}{\sinh \xi} \exp\left(\frac{-\pi}{\omega_c \tau_q}\right) \quad (3-8)$$

The period of the oscillations $1/B$ depends only upon the sheet density of the 2DCG and the magnetic field, so the sheet density of the 2DCG can be measured from the period of the oscillations. When the oscillations are plotted vs $1/B$ they are periodic. This period is

$$2\pi = \left(\frac{2\pi^2 \hbar n_s}{e}\right) \Delta\left(\frac{1}{B}\right) \quad (3-9)$$

The free carrier density, n_s , can therefore be found from Eq. (3-9). $\Delta(1/B)$ is the period of the oscillations when ρ_{xx} plotted vs. $1/B$ (Figure 3.6). Rearranging gives

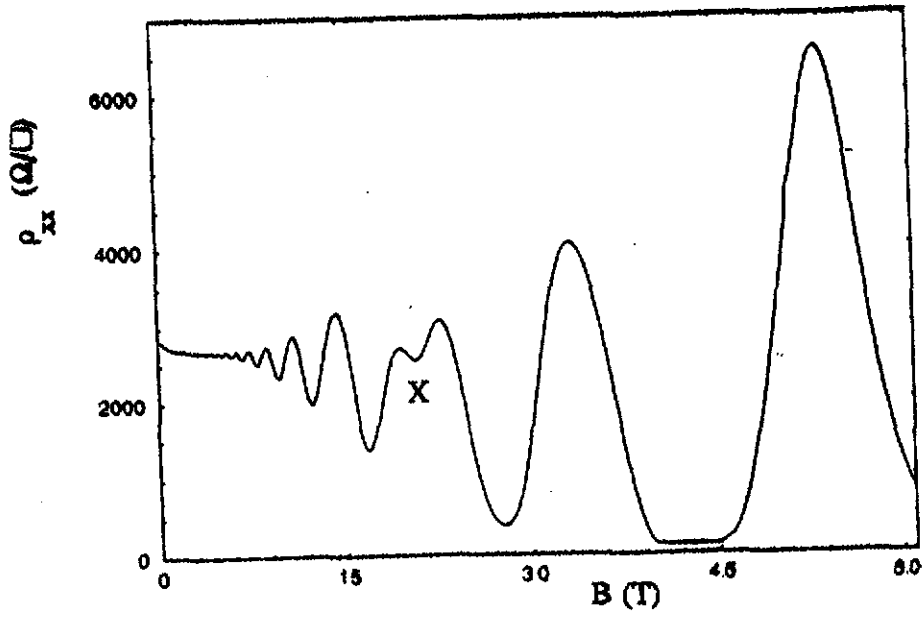


Figure 3.5: Shubnikov de Haas oscillations of magnetoresistance for sample 31.18 ($x=0.12$, $n_s=2.05 \times 10^{11} \text{ cm}^{-2}$) at 0.33 K. The point X is where spin-splitting is beginning to occur (After Plews, 1996).

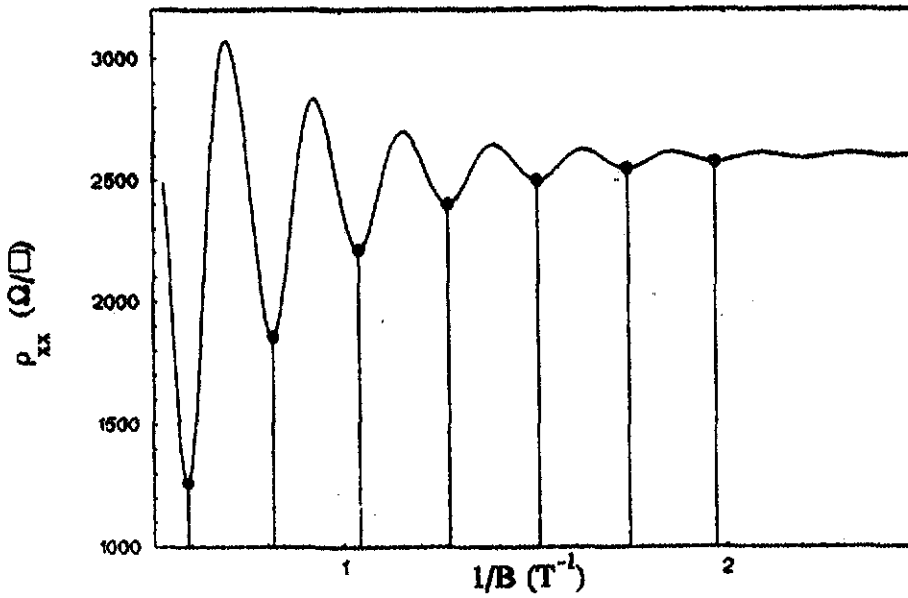


Figure 3.6: Shubnikov de Haas oscillations of magnetoresistance as a function of $1/B$.

$$n_s = \left(\frac{e}{\pi \hbar \Delta (1/B)} \right) \quad (3-10)$$

The hole effective mass and quantum lifetime are extracted from temperature dependence of amplitude of the maxima of SdH oscillations.

3.5 Thermal conductivity and thermopower measurements

There are many acceptable methods for the measurement of thermopower and thermal conductivity of materials. The widely used method is the 'Linear Heat Flow' through a sample with its ends held at two temperatures in a vacuum.

3.5.1 Sample design

The materials for this work have been grown in the Semiconductor Group of the Physics Department (University of Warwick), using solid source Molecular Beam Epitaxy (MBE) (in a VG Semicon V90S UHV system) on (001)Si substrates with 4 inch diameter. Samples were cleaved by hand. Ohmic potential contacts were made with evaporated strips of aluminium, of width $w=0.5$ mm and separated by 12 mm, which were annealed at 450-500 °C for 30-80 minutes. In order to obtain the maximum temperature difference between contacts, the sample had to be as long as possible. Samples were diamond-sawn into rectangular parallelepipeds (2.5 mm x 21 mm). The ohmic quality of Al

contacts were checked by analysing current-voltage characteristics at $T=300$ K with the help of Hewlett Packard 4145B Semiconductor Parameter Analyser.

3.5.2 Cryostat design

The design of the cryostat was based on the desirability of carrying out measurements of thermal conductivity and thermopower on the sample during one cryogenic temperature cycle. This fully welded stainless steel cryostat has been built in the mechanical workshop of Warwick University Physics Department. So, the poor thermal conductivity of the stainless steel was utilised to reduce the heat influx to the refrigerant. The vacuum junctions were reduced as much as possible in the design (vacuum seals are used successfully).

Measuring apparatus was specified for low electrical noise. Pumping and temperature control systems were carefully designed to achieve the lowest temperature; approximately $T=1.4$ K. Temperatures in the range of 1.4 K to 4.2 K were obtained by pumping in ^4He space. The cryostat design is shown in **Figure 3.7**. Noise in the measuring circuit may originate from other sources such as electrochemical effects at junctions between similar or dissimilar metals. In the experiments, 'Edwards' rotary (pressure: 1.0×10^{-2} mbar) and Turbo pumps (pressure: 1×10^{-6} mbar) were used. Vacuum pumps can cause acoustic noise and therefore should be electrically isolated from the cryostat. The cryostat has an outer shield with $T \sim 77$ K connected to liquid nitrogen bath, filled with 700 ml of liquid nitrogen, an inner bath for liquid helium (or nitrogen) of capacity 300 ml. Both these insulator jackets are covered with super isolation film to reach

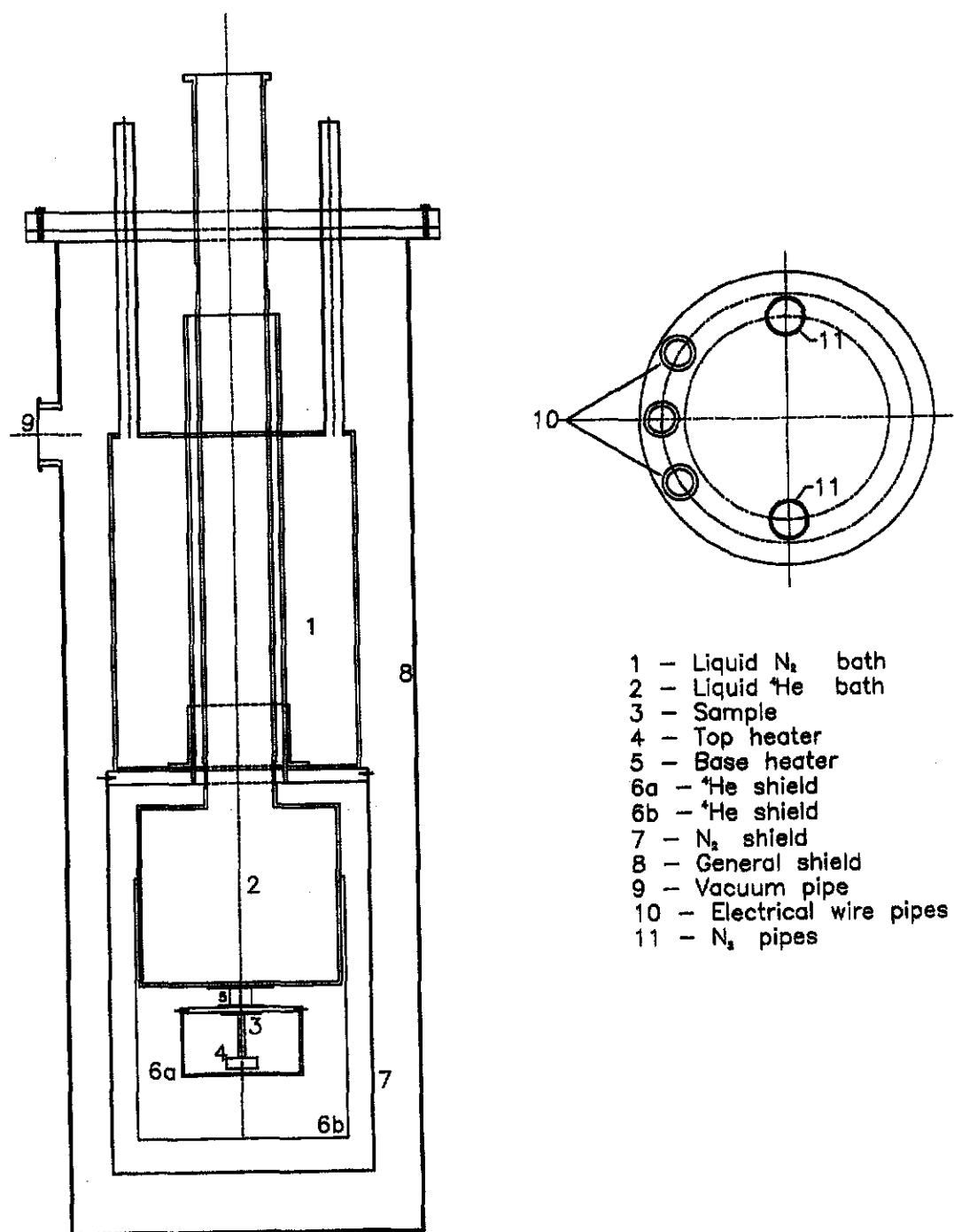


Figure 3.7: The cryostat used for thermopower and thermal conductivity measurements.

maximum using time. The liquid nitrogen hold time is 10 hours while the helium hold time is 2.5 hours. During pumping the lowest base temperature is 1.4 K with liquid helium inside the inner bath and 45 K with liquid nitrogen.

A completely insulated vacuum around the sample reduces heat loss. All heat generated in the sample heater then must flow through the sample only, enabling the calculation of thermal conductivity. Since there is an input of heat, this contact must be very efficient in order to obtain reasonably low measurement temperatures. The overall sample temperature must be controllable above the bath temperature and a 'weak link' (between sample platform and Helium bath) is therefore necessary. A copper platform support was used and it was enough to ensure adequate temperature control of the sample platform via the manganin resistance heater.

Adequate cooling power and maximum possible temperature range, which completely insulated the vacuum for the sample space and which minimised radioactive heat loss/gain of the sample, were successfully managed during the measurements.

3.5.3 Sample holder

Samples are mechanically self supporting in the cryostat. Samples are glued with silver paint to the copper support on the sample holder. Silver paint provides a reasonably good thermal contact and takes part of the strain due to the difference in thermal expansion, thus preventing the sample from breaking off during cool down.

Since the sample has to be in a vacuum to ensure a uniform temperature gradient, the sample holder is designed so that it places the sample in the inner vacuum space underneath ^4He jacket. The inner diameter of the vacuum can is 28 mm. Allowing for a 5 mm clearance around the sample, it leaves an effective space for the experiment (see **Figure 3.8 a,b**).

A strain gauge heater is glued directly to the other end of the sample. Although strain gauge is developed for a completely different reason, it is ideal for our purpose. It consists of grids of constantan on a thin polyimide supporting film (Strain gauge RS 632-124). Its resistance is nearly temperature independent at low temperatures (given in **Figure 3.9**). The function of the insert was to convey wires from the device, the heaters and the thermometers outside the cryostat and to support the sample which was suspended in a vacuum but thermally linked to the He^4 bath via a Cu block. Base temperature was controlled by a $50\ \Omega$ resistance heater connected to the temperature controller.

3.5.4 Wiring, shielding, grounding and filtering

Contacts to the top heater were made of $60\ \mu\text{m}$ diameter Au-coated Mo wires to the top heater (1,2 in **Figure 3.8**). Those to the samples were made of $100\ \mu\text{m}$ manganin (alloy: 86%Cu + 12%Mn + 2%Ni) wires (others in **Figure 3.8**), for electrical contact with poor thermal conductivity (**Figure 3.10**). Therefore there was no significant heat leak from the sample due to wiring. The wiring was carried out using twisted pairs of 100 micron manganin wires; the wiring for thermometers consisted of double twisted pairs enabling 4-point

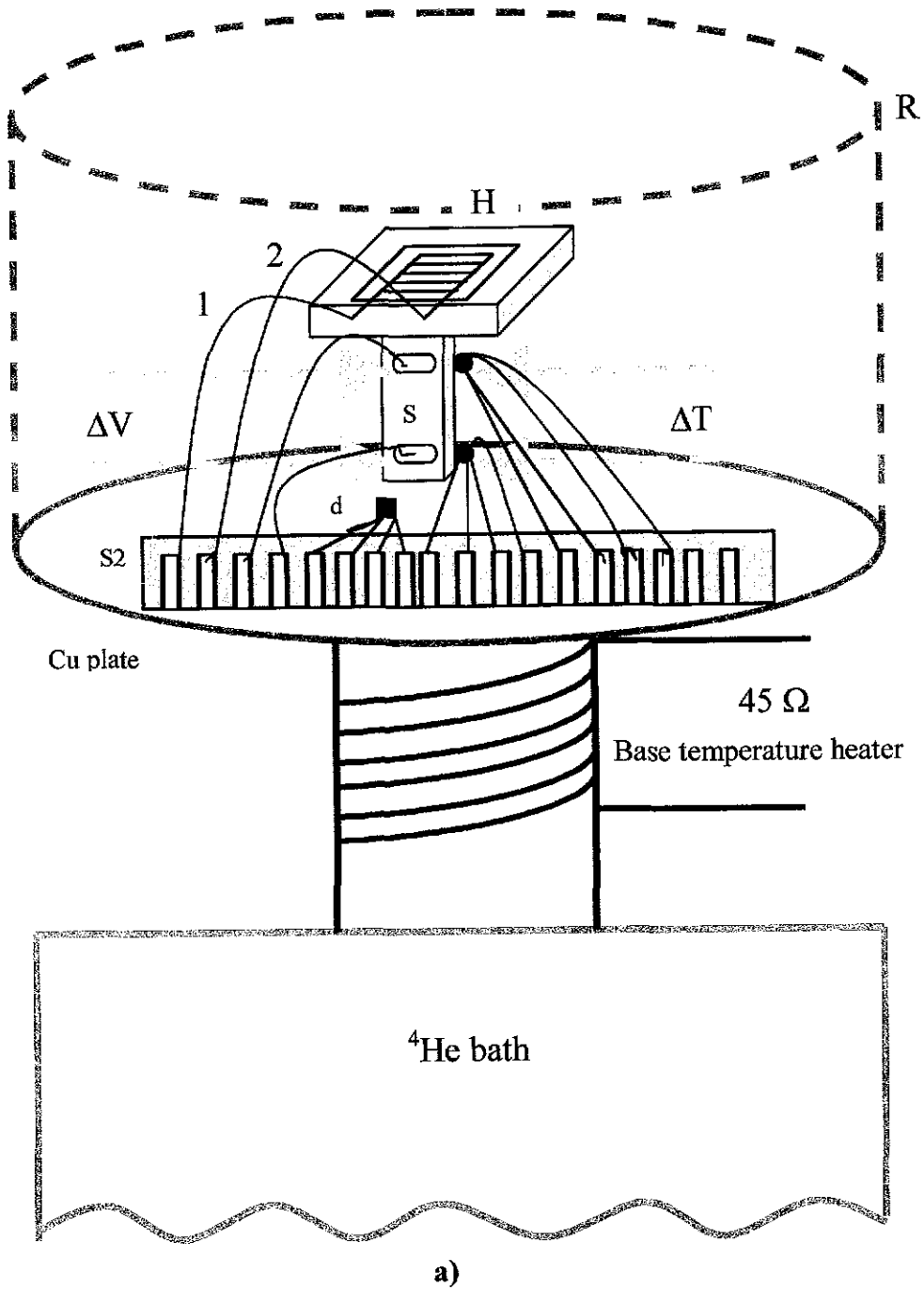


Figure 3.8: Sample holder: S is sample, H is a strain gauge heater (resistance: $120\ \Omega$) mounted on a Cu block, R is a low temperature shield and d is a Si-diode.



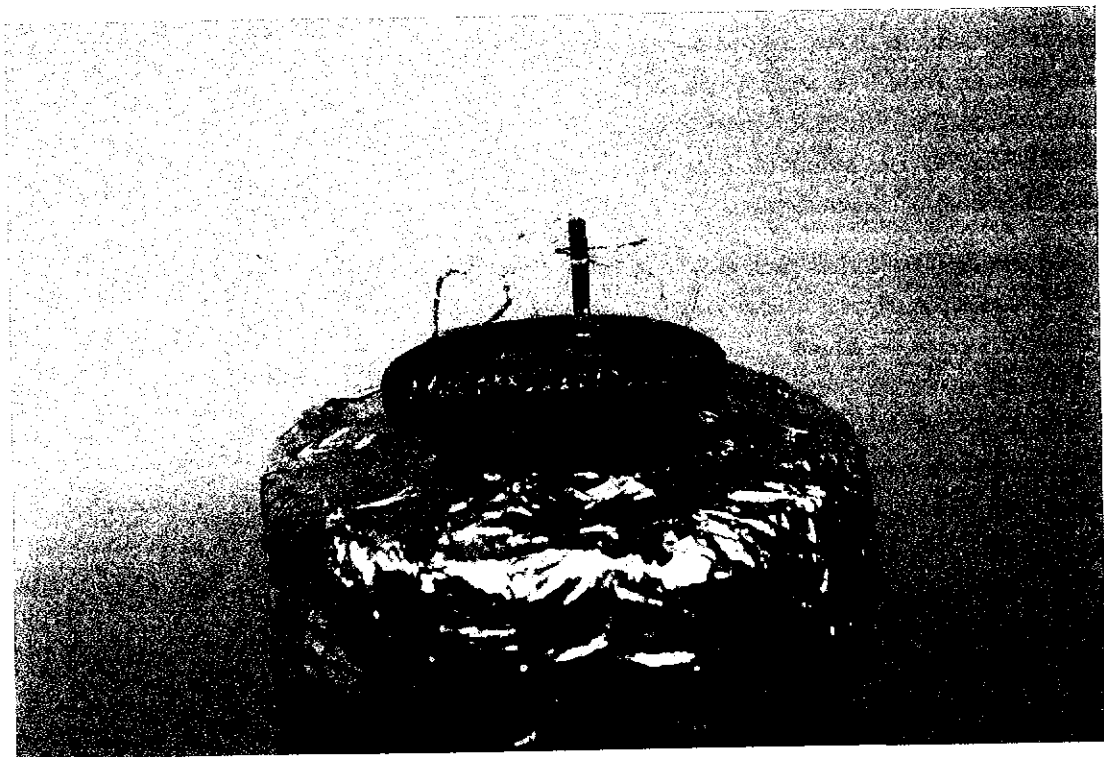


Figure 3.8 (b): Photographs are taken from the sample holder part of the cryostat.

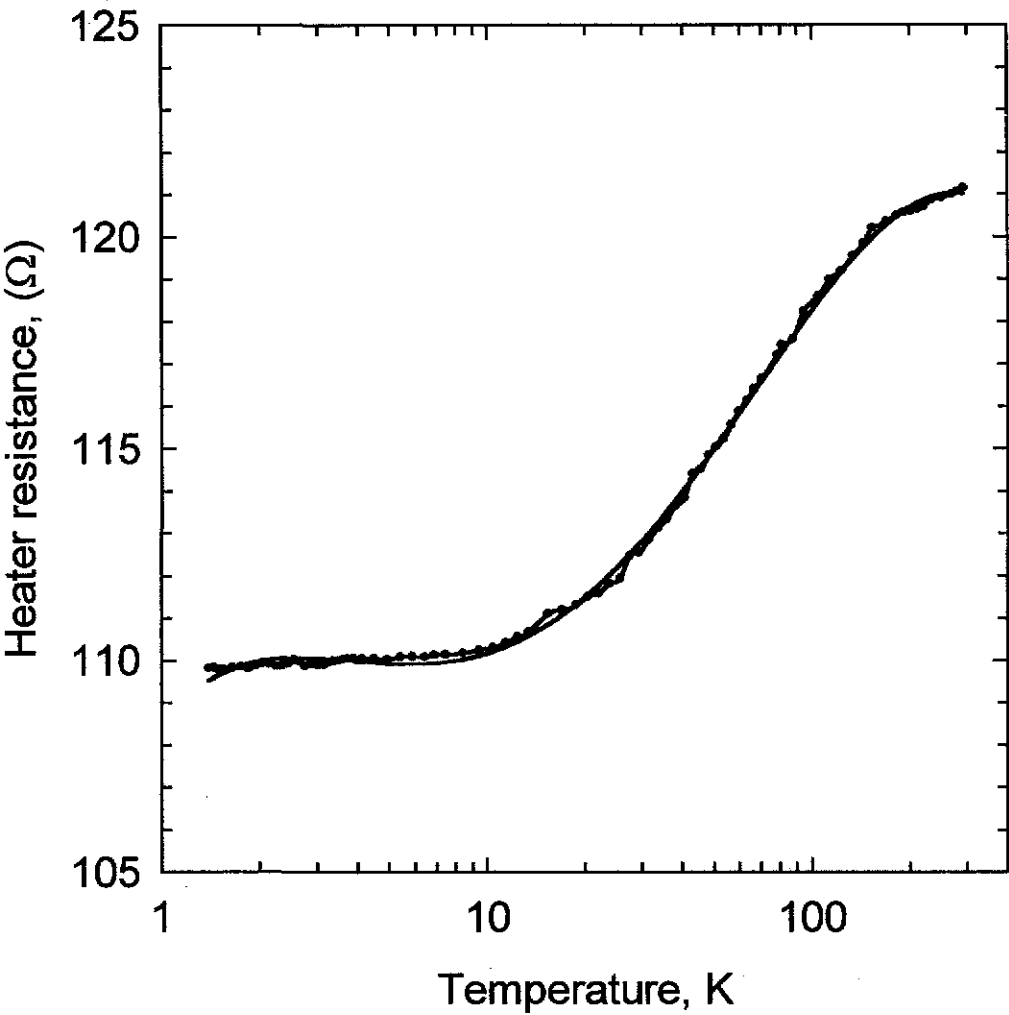


Figure 3.9: The calibration of strain gauge heater used during the measurements.

measurements. The thermoelectric power of manganin (given **Figure 3.11**), which has to be considered due to the temperature differences of the contacts, is negligible compared to the thermopower of the 2DHG.

The small diameter results in a very large thermal resistance for the wiring. Typically the wiring conducts around 0.3% of the heat input at the top heater (H). By thermal anchoring of the wiring to S2 (**Figure 3.8 a**) and subsequent temperature control of the sample base temperature, the amount of heat conducted along the wiring should prevent heat escaping or entering the sample. All wires were connected between the wiring sink and the heater (base heater) block. Two of these were for the heater, as normal and two were for a thermometer attached by silver paint to the heater block, as with a normal sample.

Laboratories and cryostats are electrically noisy environments with the isolation and shielding. Stray magnetic fields from rotary pumps, leakage currents from diffusion-pump heaters and cheap switched-mode power supplies in computers can all cause currents that circulate round the wiring and pipe work and might interfere with the experiment. To overcome this problem, all leads have been filtered into the cryostat place.

3.5.5 Thermal contact and heat transfer

It needs great care to ensure adequate thermal contact between the sample, heater, sink and thermometers. These contacts have been experimentally

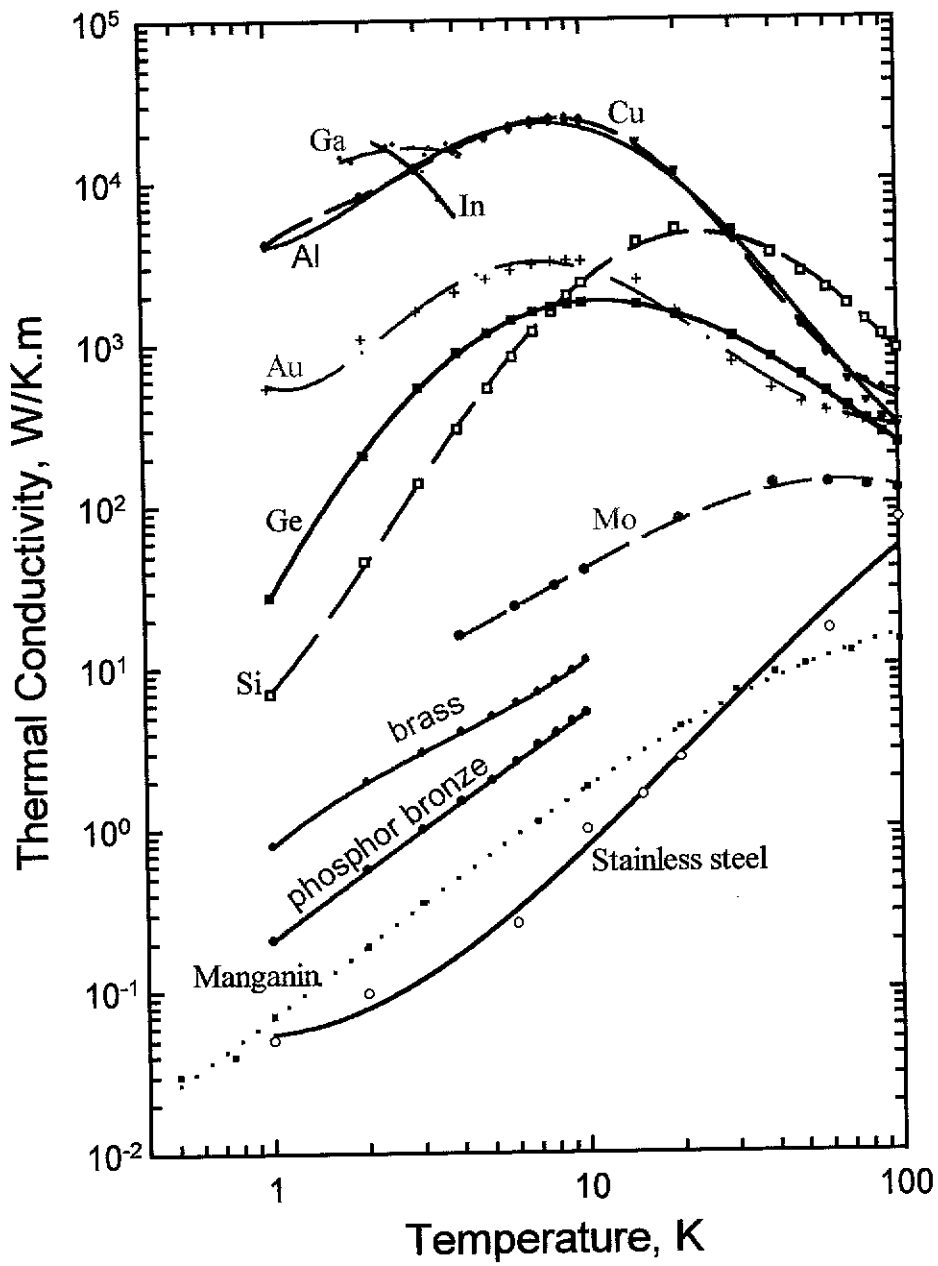


Figure 3.10: The measured thermal conductivities as a function of temperature with various metals and semiconductors. Taken from:

(Al, Au, Cu, Ge and Si): Lide, (1999).

(Ga, In and stainless steel): Childs, Ericks and Powell (1973).

(Mo): Powell, Harden and Gibson, (1960).

(brass, phosphor bronze and manganin): LakeShore (2000).

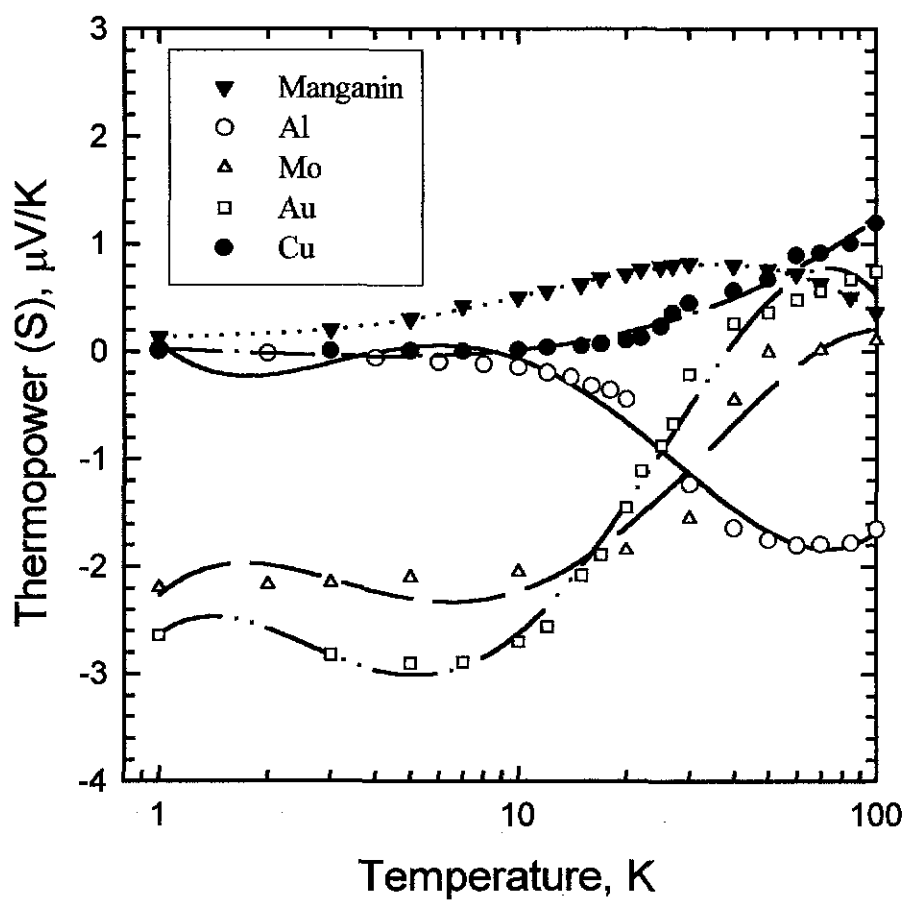


Figure 3.11: Temperature dependence of absolute thermopower of metals which are used during measurements. (Taken from: manganin: Rathnayaka, 1985 and Al, Mo and Au: Rowe 1995).

and theoretically characterised. There was reduced heat loss from H down the heater wiring. Radiative heat transfer between the sample and various elevated temperature areas was eliminated by the installation of temperature controlled radiation shield, R (**Figure 3.8 b**).

There is a range of measurement currents for the thermometers that ensures a negligible heating effect. All measurements were made within these conditions. In fact, since the sensors are calibrated for each measurement point, the effect of overheating, provided it is not large, is automatically taken into account since calibration is made when both measurement currents are on. If the heating current is low, then little heat transfer to the sample will take place either.

The basic principle underlying the measurement of thermoelectric power is to apply a temperature gradient to a device and to measure the resulting voltage. For thermopower measurements at low temperatures, a good thermal joint to a cold sink is needed at one end and to a heater on the other end of the sample. The sample has to be in vacuum to maintain a uniform temperature gradient.

3.5.6 Measuring temperature gradient

To obtain reliable absolute values for the thermopower, an accurate knowledge of temperature and temperature gradient is essential. For this purpose, two resistance thermometers were glued directly to the backside of the substrate. To measure ΔT , thick film carbon (C) temperature sensors (in **Figure**

3.8) were attached to the sample using a colloidal silver adhesive (RS 552-494). The sample (**Figure 3.8**) was mounted to the copper block using the same adhesive. Alternative thin film germanium (Ge) temperature sensors were used. The package size of the carbon temperature sensor was $(4 \times 1.5 \times 0.55)$ mm of sapphire substrate and “ARALDITE” epoxy resin cover, while the actual device size of carbon-paper was $0.5\text{mm} \times 0.5\text{mm} \times 80\mu\text{m}$. On the other hand, the package size of a temperature sensitive crystal consisting of the chip of p-Ge($2\mu\text{m}$)/i-GaAs (0.2mm) heterostructure with $(0.5 \times 0.5 \times 0.2)$ mm is $(3 \times 1.5 \times 1.5)$ mm. The current through the temperature sensors was 10^{-3} - 10^{-6} A at ≈ 300 -1.4 K, respectively.

To measure base temperature, a ‘Lakeshore’ DT-470 silicon diode thermometer was mounted on a Cu flat surface by applying silver adhesive. This fast responding sensor is useful where there are space constraints and where a wide range of temperatures are desired. Using a constant current of $10\mu\text{A}$, the forward voltage from the diode changed from about 1.8 V at 1.4 K to 0.5 V at 300 K. Its size was 2×2 mm. Accuracy of the Si diode calibration thermometer was ± 10 mK between 1.4-300 K temperatures.

Thick film carbon (C) temperature sensors and thin film Ge temperature sensors were used to measure the temperature difference between two points of the sample at a distance of 12 mm. **Figure 3-12** shows resistance (R) vs. temperature and **Figure 3.13** shows sensitivity vs. temperature for temperature sensors and the Si diode thermometer which were used in the experiments. Sensitivity was defined as follows:

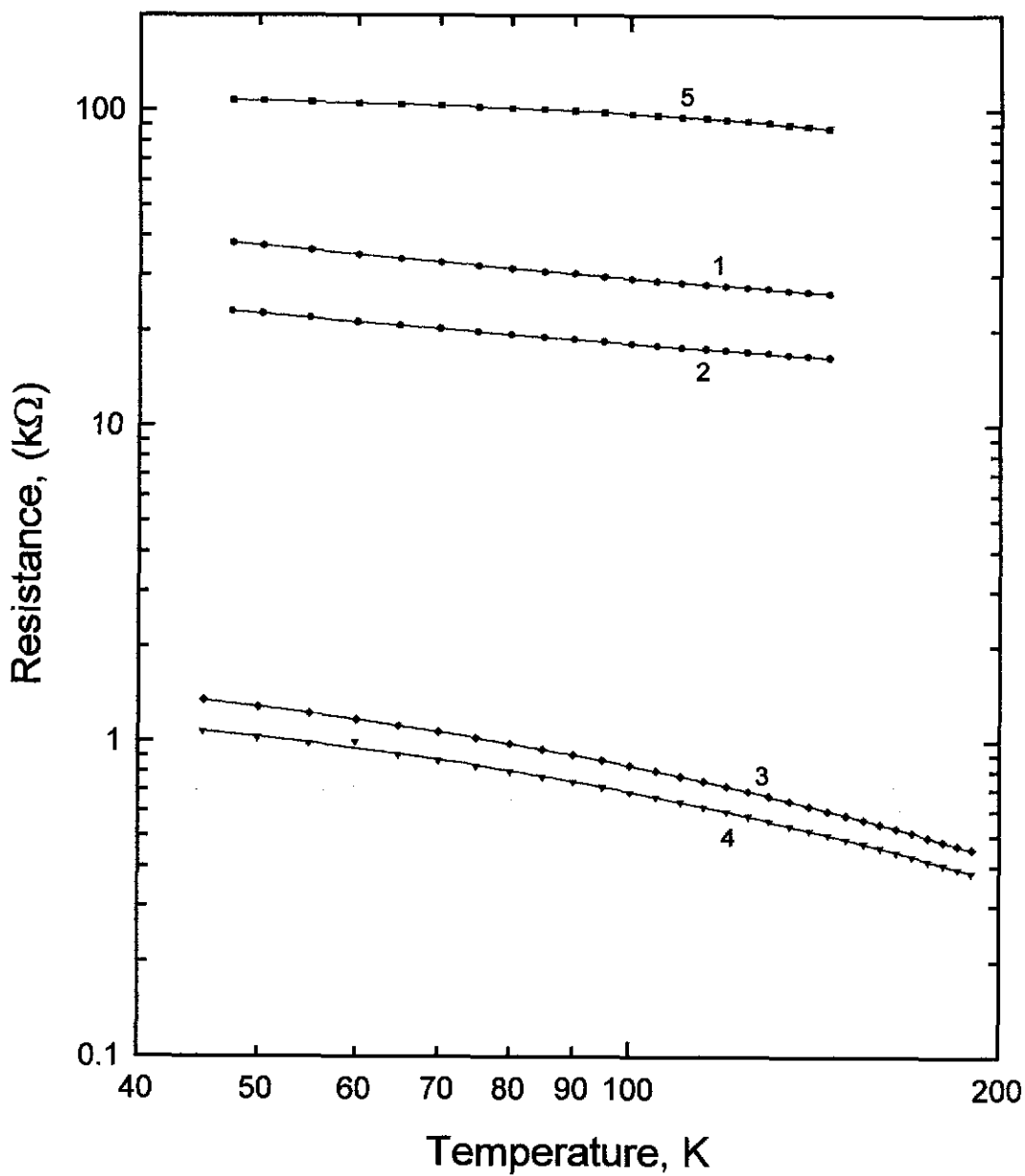


Figure 3.12: Temperature dependence of resistance of thick film carbon (C) (1, 2) and thin film germanium (Ge) (3, 4) temperature sensors and silicon (Si) diode thermometer (5).

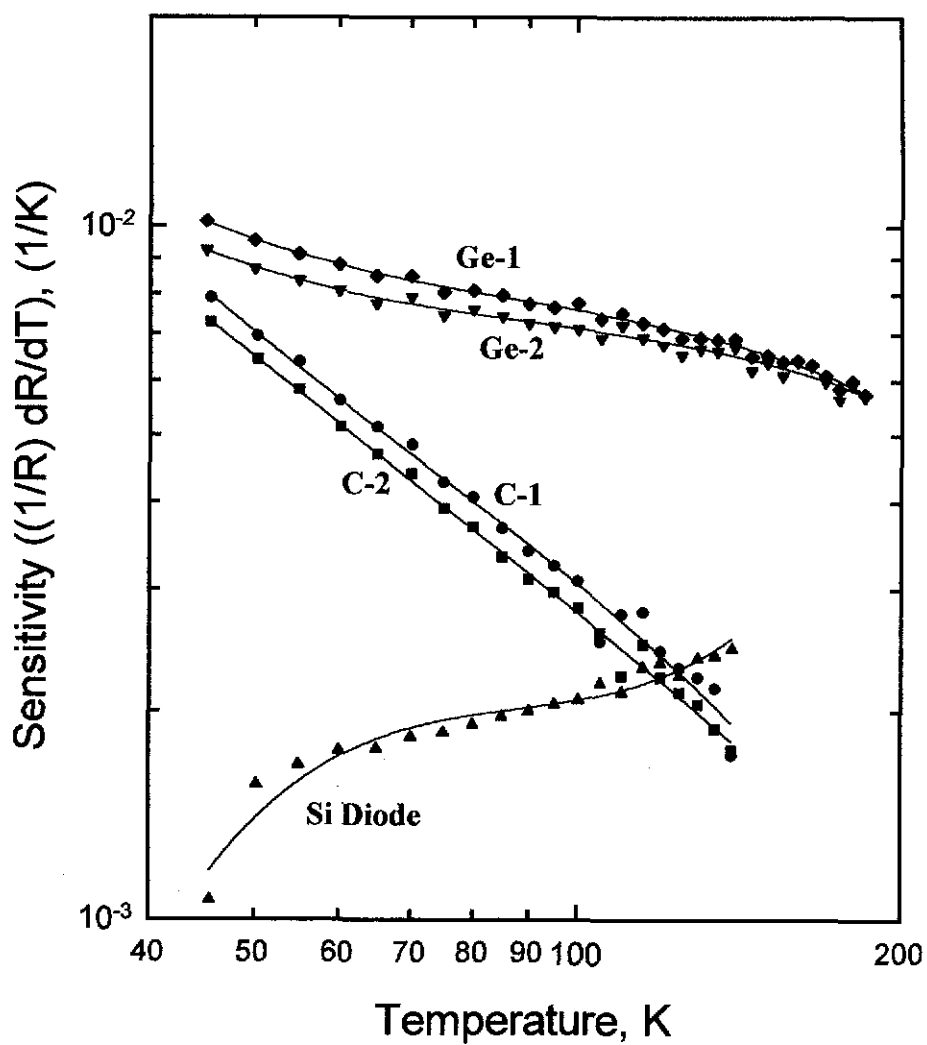


Figure 3.13: Temperature dependence of sensitivity of carbon (C-1, C-2) and germanium (Ge-1, Ge-2) temperature sensors and silicon (Si) diode thermometer.

$$\text{Sensitivity} = \frac{1}{R} \frac{dR}{dT} \quad (3-11)$$

These figures show that thin film Ge temperature sensors have lower resistance and more sensitivity than carbon sensors and the Si diode thermometer at T=300-45 K, for resistance falls rapidly with increasing temperature. Although there is high sensitivity at low temperatures it falls off at high temperature. Suitable models can be used down to 50 mK, and others up to 30 (or even 100) K. **Figure 3.14** shows calibration of these Ge sensors' dependence on temperature. In order to obtain stable temperature and voltage conditions, it was necessary to wait a few seconds for He temperatures measurements. It was necessary to wait approximately 20 minutes at nitrogen temperatures after applying the heater current or changing the base temperature. Measurements at low temperature are difficult. Good thermal contact and the minimisation of self-heating are necessary. In this work, as the samples were small, (0.5x2.5x21) mm, it was necessary to use a small thermometer. Resistance thermometers can be manufactured on a micro scale. The thermometer material should be chosen so as to offer the least resistance whilst still possessing a large change in resistance per unit temperature.

The use of a sapphire substrate for the germanium film, combined with epoxy paint adhesive for the film to sapphire joint and the sapphire to sample contact, ensures good thermal contact to the sample. Being a good thermal conductor, the sapphire substrate also provides extremely good electrical isolation between the thermometer resistance measuring circuit and the sample.

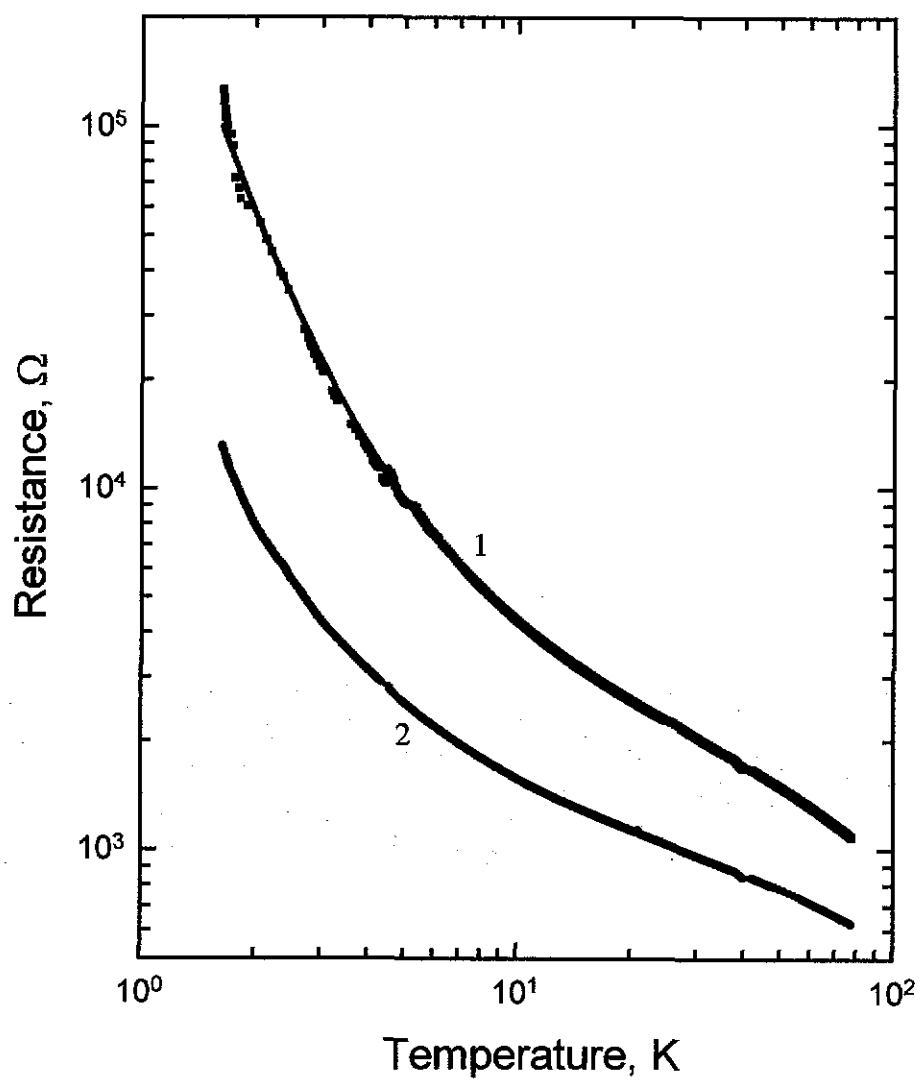


Figure 3.14: Resistance vs. temperature of two Ge temperature sensors (1 and 2).

3.5.7 Measuring voltage

The voltages associated with the thermoelectric effect are usually small. In the course of this work they have usually been in the range of $0.1\ \mu\text{V}$ to $100\ \mu\text{V}$. As described above, the temperature difference could only be accurately determined for a constant heat current, i.e. a d.c. electric supply to the heater resistor. This entailed, therefore, doing d.c. measurements to obtain the thermoelectric emf and the thermopower. A Keithley 181 nanovoltmeter was used for this purpose. This has an input impedance of more than $1\ \text{G}\Omega$ and isolated from the earth.

It can be seen that the ground connection to the sample was made at the nanovoltmeter, which was partly due to the fact that the first nanovoltmeter cable used had a short between input low and ground. As well as the offset current effect described above, there are other ways in which extraneous d.c. voltages can be introduced into the measuring system. First, the device can rectify radio frequency voltages picked up from the surroundings. Secondly, the bending of coaxial or triaxial cables (the triboelectric effect) can induce extra voltages. This was minimised by taping all the cables to something rigid when performing measurements. Finally, even with no power supplied to the heater resistor, the difference between reversed and unreversed voltmeter readings is non-zero (typically 1 to $2\ \mu\text{V}$). This extra voltage is due to strain and inhomogeneity in the wires down the insert and possibly the existence of a small 'extra' temperature gradient. This was allowed for by always measuring the voltage with and without a temperature gradient and then taking the difference.

At low temperature, signals of this magnitude are comparable with the fundamental noise levels of the system so it was important that external electrical interference was prevented or reduced to an acceptable level.

3.5.8 Measurement equipment

A “Keithley” 181 nanovoltmeter was used to measure thermoelectric voltages, a “Keithley” 220 programmable current source to apply current ($I=1.0$ - 30 mA) to the top heater and “Thurlby” 1905a Intelligent digital multimeters were used to obtain resistance (with measuring current $I_m=10^{-3}$ - 10^{-6} A) from the temperature sensors. The resolution of the VT measurements (due to resolution of “Thurlby” multimeter and values of resistance at **Figure 3.12** and sensitivity at **Figure 3.13**) was 7mK at 45 K ($I_m = 10^{-5}$ A) for carbon-paper sensors and 1mK for Ge thin film sensors at $T = 45$ K ($I_m = 10^{-3}$ A).

Stable base temperatures were defined using a “LakeShore” DRC-91CA Temperature Controller during the experiments for the Si-diode thermometer. Control stability of DRC-91CA Temperature Controller: within ± 1 mK below 30 K, ± 5 mK above 30 K using a diode sensor (LakeShore, 1990).

3.5.9 Experimental procedure

The experiment starts with sample installation. The sample is put to the heater, which is epoxied on the Cu block aided by silver paint. The sample is inserted into Cu block (sample holder) and everything is allowed to dry for 8-10 hours. The electrical connections are made to the distribution board by solder

bonds. Three radiation shields are attached (**Figure 3.7** (6a,6b and 7)), the outer vacuum jacket bolted on and all instruments are checked to be correctly wired up and operating. The cryostat is then pumped out with a rotary pump, and then switched to a turbo pump.

When the cryostat pressure reaches $<1 \times 10^{-4}$ mbar or less, cooling can begin. Introducing liquid nitrogen to the nitrogen bath causes this bath and the outer radiation shield to cool. Also, the pressure in the cryostat falls rapidly below 10^{-5} mbar, which is an acceptable pressure for the measurements to take place. After two or three hours, the pressure reaches to 10^{-6} mbar and then we start the experiment. The Helium bath is pre-cooled with liquid Nitrogen to approximately 80 K. During the precooling process, the sample temperature is controlled at various points between 300 and 80 K such that an initial rough characterisation of the resistivity is possible. When the temperature is 80 K, liquid Helium is introduced by a siphon. Resistivity characterisation continues in the above fashion, and the bath temperature falls to approximately 4.2 K along with pressure to a constant of the order of 1×10^{-6} mbar.

Thermopower and thermal conductivity are measured at the same time. A temperature gradient is established by exciting the top heater with a current such that the temperature gradient is approximately 50 mK. The appropriate current varies with sample thermal conductivity (and therefore temperature) and is judged by experience. The exact temperature gradient is unimportant as the thermal voltage and temperature gradient are linearly dependent on heating power (as will be shown in section 4.4). Although one temperature gradient is all

that is necessary, the gradients of $\Delta V/\Delta T$ and ΔT vs. power are checked often throughout the course of the measurements to ensure that there are no errors in the measurements.

It is important to wait for a considerable amount of time for thermal equilibrium to be thoroughly established. At liquid Helium temperatures the procedure is then to note the sample base temperature, both thermometers' resistances, the heater current and the thermoelectric voltage. Before and after applying the direct current, the sample base temperature is noted, as well as the both of the thermometer resistances and the thermal voltage (for offset calculation purposes). The temperatures of the upper and lower thermometers during heating may then be calculated, the actual thermal voltage determined and the thermopower and thermal conductivity calculated. The procedure is then repeated for another temperature point.

CHAPTER FOUR

RESULTS FOR MBE AND CVD GROWN SiGe/Si TWO DIMENSIONAL STRUCTURES

4.1 Introduction

In recent years, there has been much interest in the properties of two dimensional electron and hole systems. The first part of this chapter presents the transport properties of a two-dimensional hole gases (2DHGs) studied at inverted and normal interface of a strained $\text{Si}_{0.8}\text{Ge}_{0.2}$ quantum well. The second part presents the measurements of the temperature dependence of the thermopower and thermal conductivity in 2DHGs heterojunctions and in a high mobility 2DEG sample. Also, in this chapter, a comparison of the present results with the established theory and other experimental works is made. Theory and previous experimental work on two dimensional thermopower were presented in Chapter 2. In this chapter, we present only the results for the 2DHG and 2DEG Si/SiGe samples. Also presented in this chapter are results for simple doped epilayer structures which help to clarify various aspects of the results on the 2DHGs.

4.2 Hall effect measurements

The low temperature transport properties of modulation doped two dimensional hole gas structures have been a subject of great interest in the past for physics and device applications (Whall *et al.*, 1995; Lander *et al.*, 1997; Sadeghzadeh, 2000). In these structures, a quasi-two dimensional hole gas (2DHG) was formed in the $\text{Si}_{0.8}\text{Ge}_{0.2}$ quantum wells with 4.2 K sheet carrier densities measured in the range $(2.5\text{-}6.5)\times 10^{11} \text{ cm}^{-2}$. The samples were also characterised by x-ray diffraction (XRD) and Shubnikov de Haas (SdH) measurements. The temperature dependence of the specimens' resistivity, mobility and sheet carrier density were determined using Hall and van der Pauw measurements on Greek cross mesa structure. Ohmic contacts were formed by Al into the structures. The measurements were carried out in a lattice temperature range between 1.5 K and 300 K in Cryostats.

Figure 4.1 shows the temperature dependence of the carrier density n_s of some normal and inverted samples. The Hall measurements provide information about total sheet carrier concentration n_{Hall} and Hall mobility μ_{Hall} . As seen from this figure all samples show almost the same characteristics. The carrier densities remain constant up to lattice temperature 60 K and 100 K (sample 56.15). However, above these temperatures the hole densities increase monotonically with temperature for all samples probably because of the temperature induced thermal excitation of impurities (B) in the $\text{Si}_{1-x}\text{Ge}_x$ region. The flat region below these temperatures implies that the conduction is dominated almost exclusively by the carriers in the wells. The parallel conducting channel contributing to the

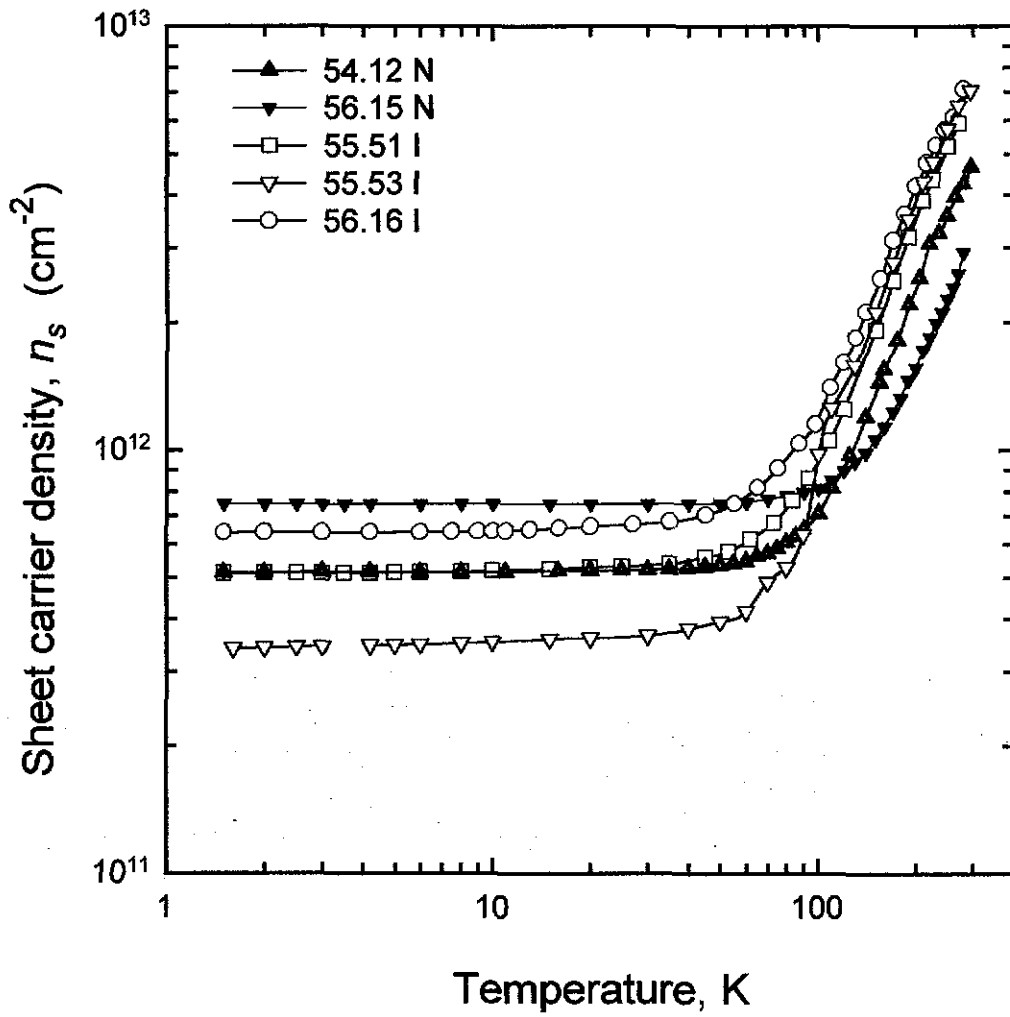


Figure 4.1: Total sheet hole density as a function of lattice temperature obtained from Hall and Van der Pauw measurement techniques for normal (N) and inverted (I) samples.

major conduction channel in the wells will be discussed later during analysis of the results. Hole mobility remains almost constant from 1.5 K up to 10 K (Figure 4.2). Figure 4.3 illustrates temperature dependence of resistivity for the same samples.

Figure 4.4. shows the temperature dependence of resistivity (ρ), mobility (μ) and sheet carrier density (n_s) for a Si/Si:B/Si structure. These were determined using van der Pauw measurements on Greek cross mesa structure to characterise the epilayer sample 50.36. The difference in electrical properties of a modulation doped and a simple doped structure (epilayer) can be understood by comparing the experimental results shown in Figures 4.1-3. In the simple doped structure, the resistivity decreases with increasing temperature (see Figure 4.4). Around liquid nitrogen temperature (77 K), most of the holes associated with boron dopants freeze out and the sample has a huge resistivity at very low temperatures. In contrast, the normal modulation doped structure has a resistivity at low temperatures (below 77 K). The 2DHG continues conduct giving a finite sheet resistivity. The Hall mobility which is limited by phonon scattering at room temperatures, increases with decreasing temperature in normal modulation doped structure approaching 10 000 cm²/V.s (at 1.6 K), while that of the simple doped structure has a maximum value of ~100 cm²/V.s at intermediate temperatures (~100 K), and decreases at low temperatures where hopping conduction exists. Table 4.1, 4.2 and 4.3 give a summary of the grouping of the samples into various studies which were possible. As a doped layer is grown at some distance below the conduction channel, any migration

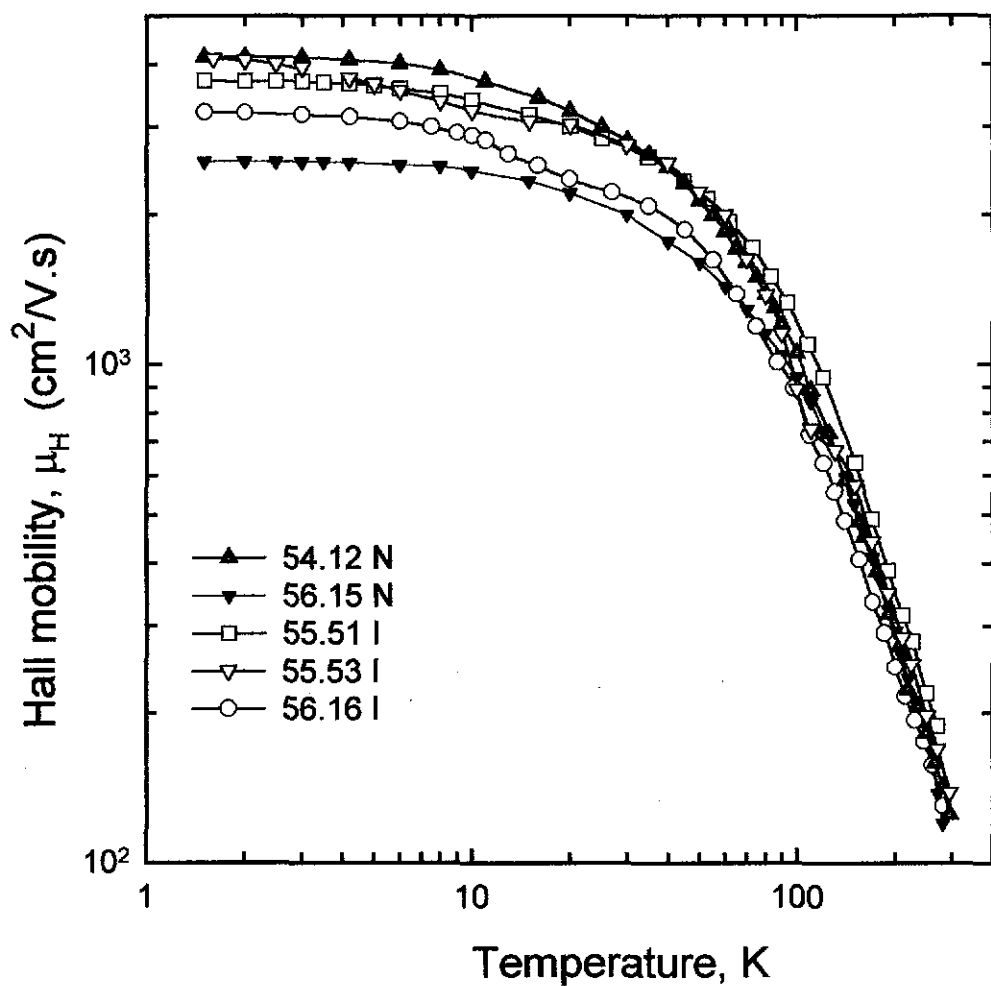


Figure 4.2: The mobility as a function of lattice temperature obtained from Hall and van der Pauw measurement techniques.

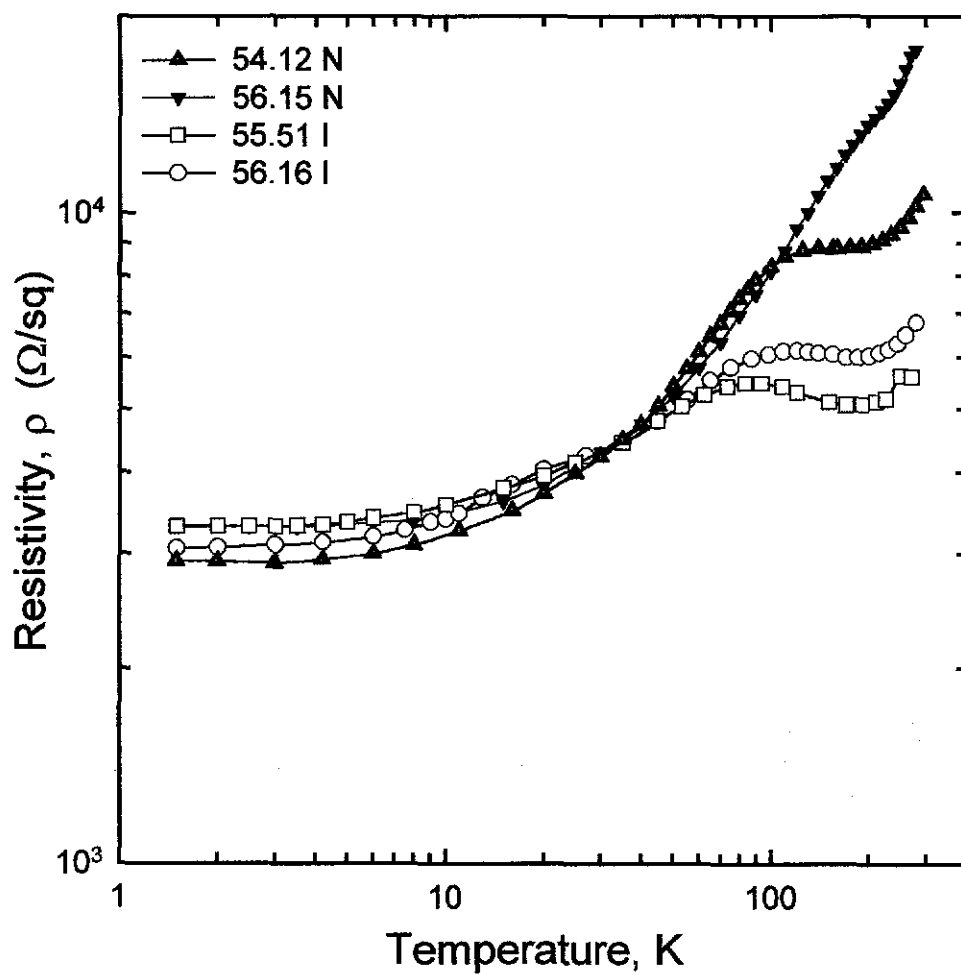


Figure 4.3: Resistivity dependent on temperature using by Van der Pauw technique.

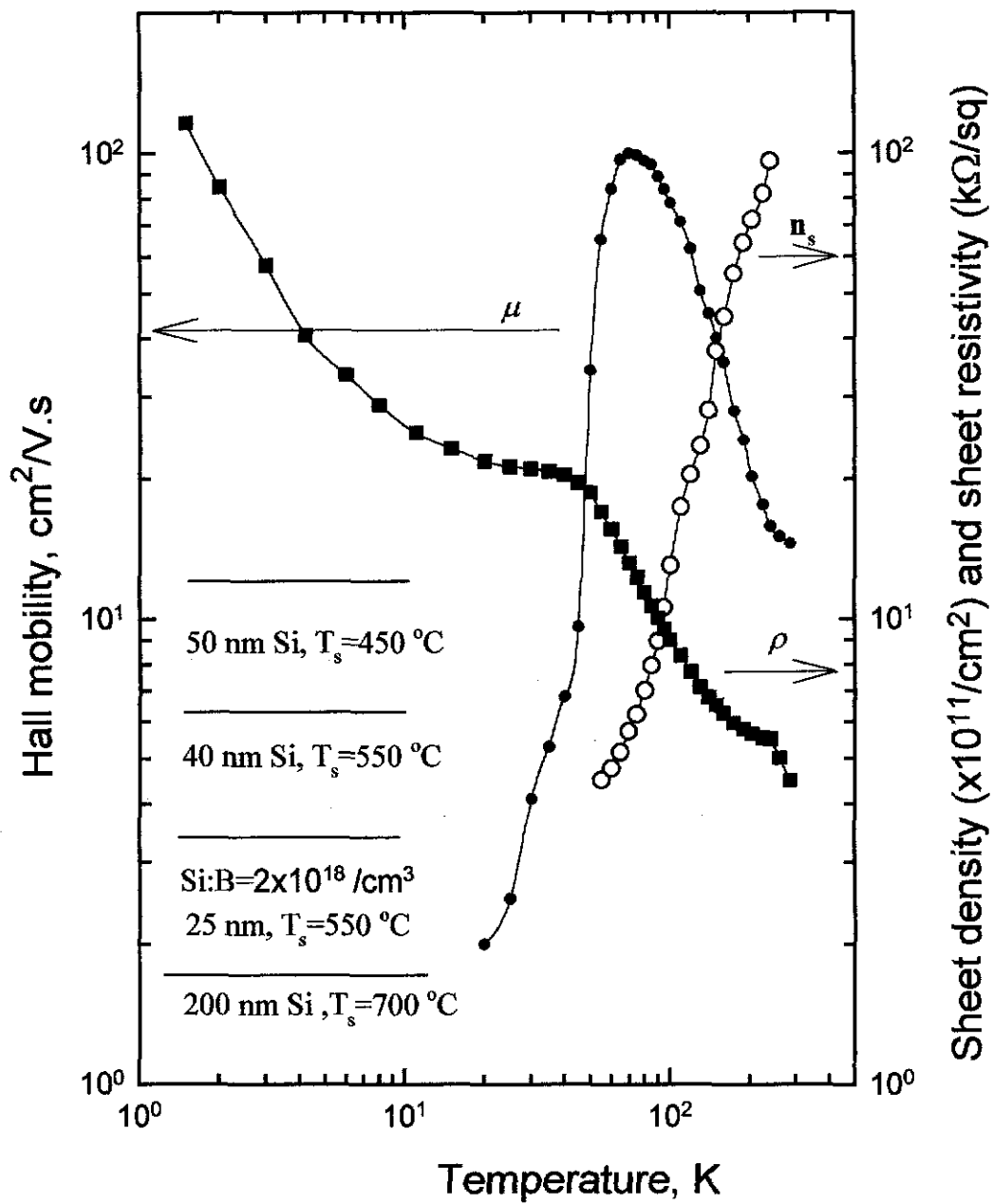


Figure 4.4: Variations of hole sheet density (open circle), resistivity (filled square) and Hall mobility (filled circle) versus temperature of a Si/Si/Si structure (sample 50.36).

(segregation) of dopant atoms into the spacer (dopant setback) and/or channel may reduce the effective spacer thickness and the 2DEG and 2DHG mobility in the channel. There has not been any report about boron segregation in ultra high vacuum chemical vapour deposition UHV-CVD (Wang *et al.*, 1989) techniques.

4.3 SdH measurements of 2DHG at the Si/SiGe/Si inverted interface

As we mentioned before Hall measurements provide information about only the total sheet carrier concentration n_{Hall} and Hall mobility μ_{Hall} . To evaluate the 2D carrier concentration per well, n_s , at the Fermi level and quantum mobility μ_q , we have used Shubnikov de Haas (SdH) method. The variation of the longitudinal resistivity ρ_{xx} (at $B=0$) with temperature for sample 55.53 is shown in **Figure 4.5**. There is no minimum of resistivity observed below 1 K usually attributed to competition of weak localisation and hole-hole interactions. The variation of sheet conductivity [$\sigma_{xx}(T)=1/\rho_{xx}(T)$] with temperature is shown inset **Figure 4.5**. Typical magnetoresistance oscillations observed in the inverted modulation doped sample 55.53 is shown in **Figure 4.6**. The 2D hole density per well can be obtained from the plots of the reciprocal magnetic field ($1/B$), at which the n_{th} peak occurs, against the peak number (n). **Figure 4.7** shows the graph of magnetoresistance versus $1/B$ (The data were taken at each minimum peaks). The 2D hole density has been calculated from this figure by using Eq. (3-10).

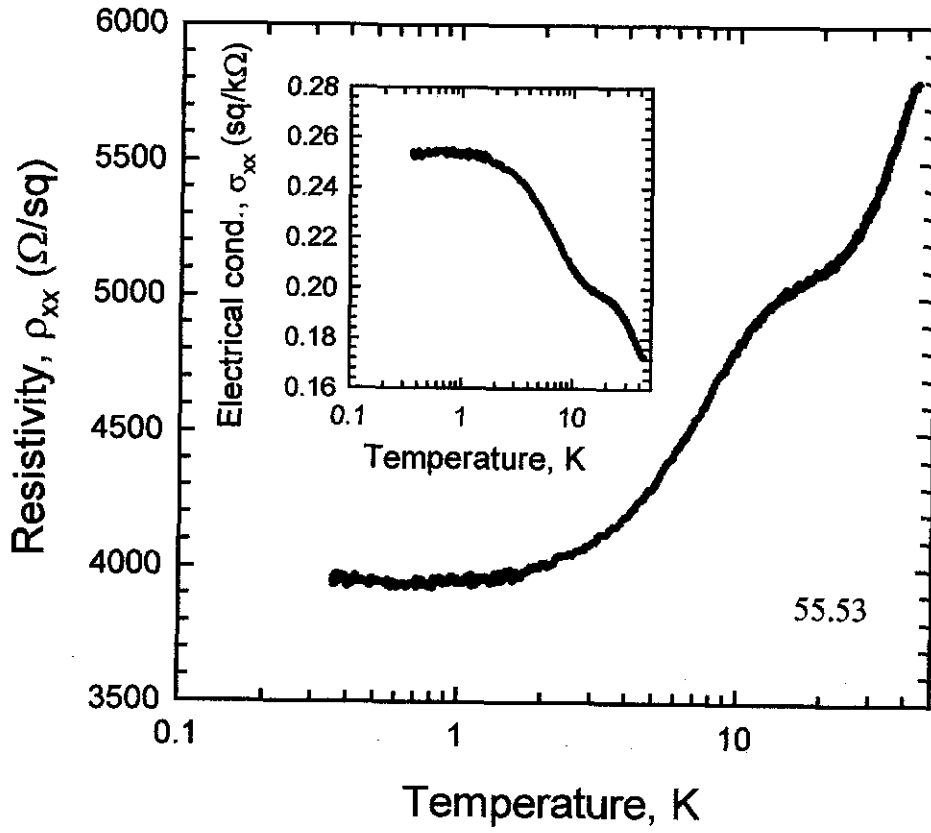


Figure 4.5: Variations of resistivity and conductivity (inset) versus temperature of inverted 2DHG sample 55.53 at $B=0$.

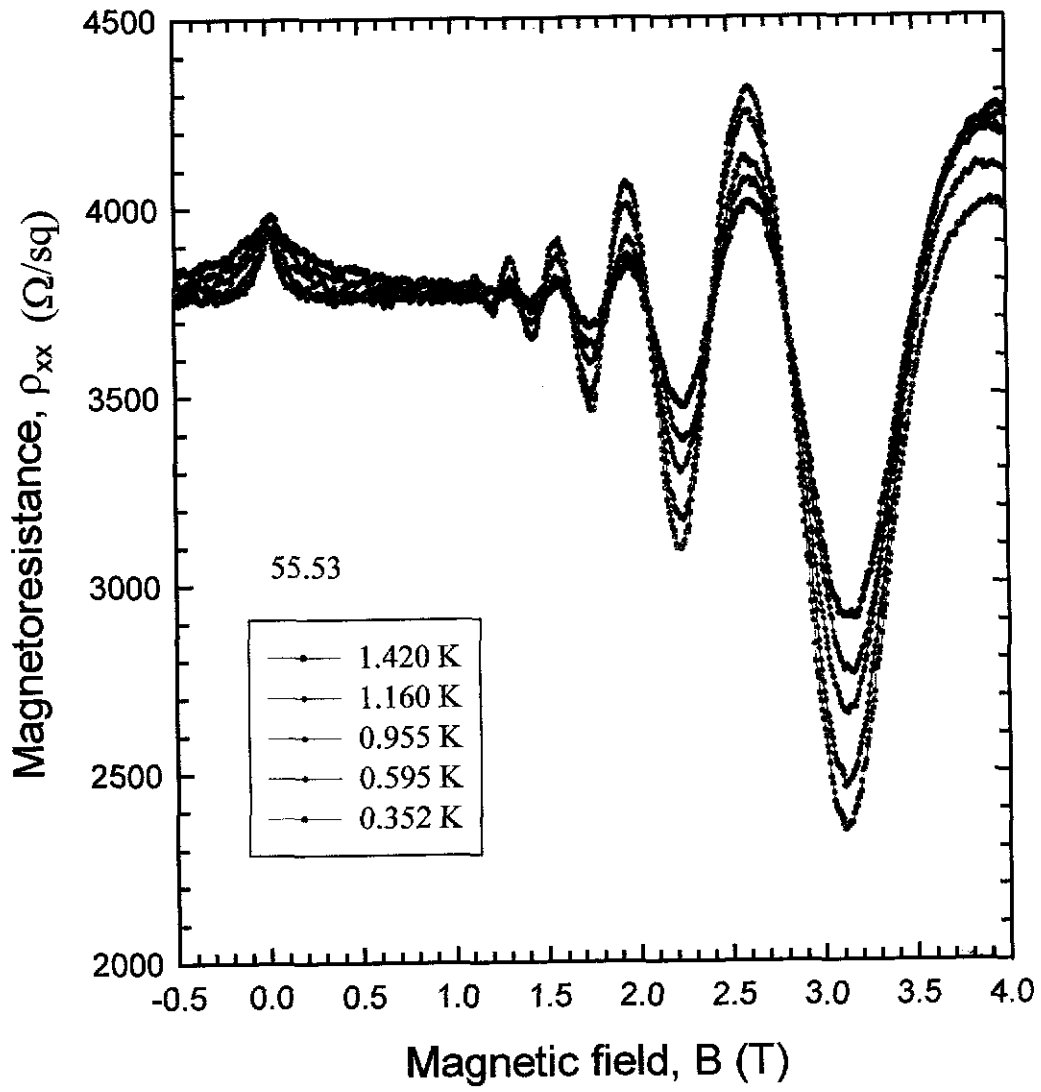


Figure 4.6: Shubnikov-de Haas oscillations of magnetoresistance for inverted 2DHG sample 55.53 ($x=0.20$, $n_s=3.8 \times 10^{11} \text{ cm}^{-2}$).

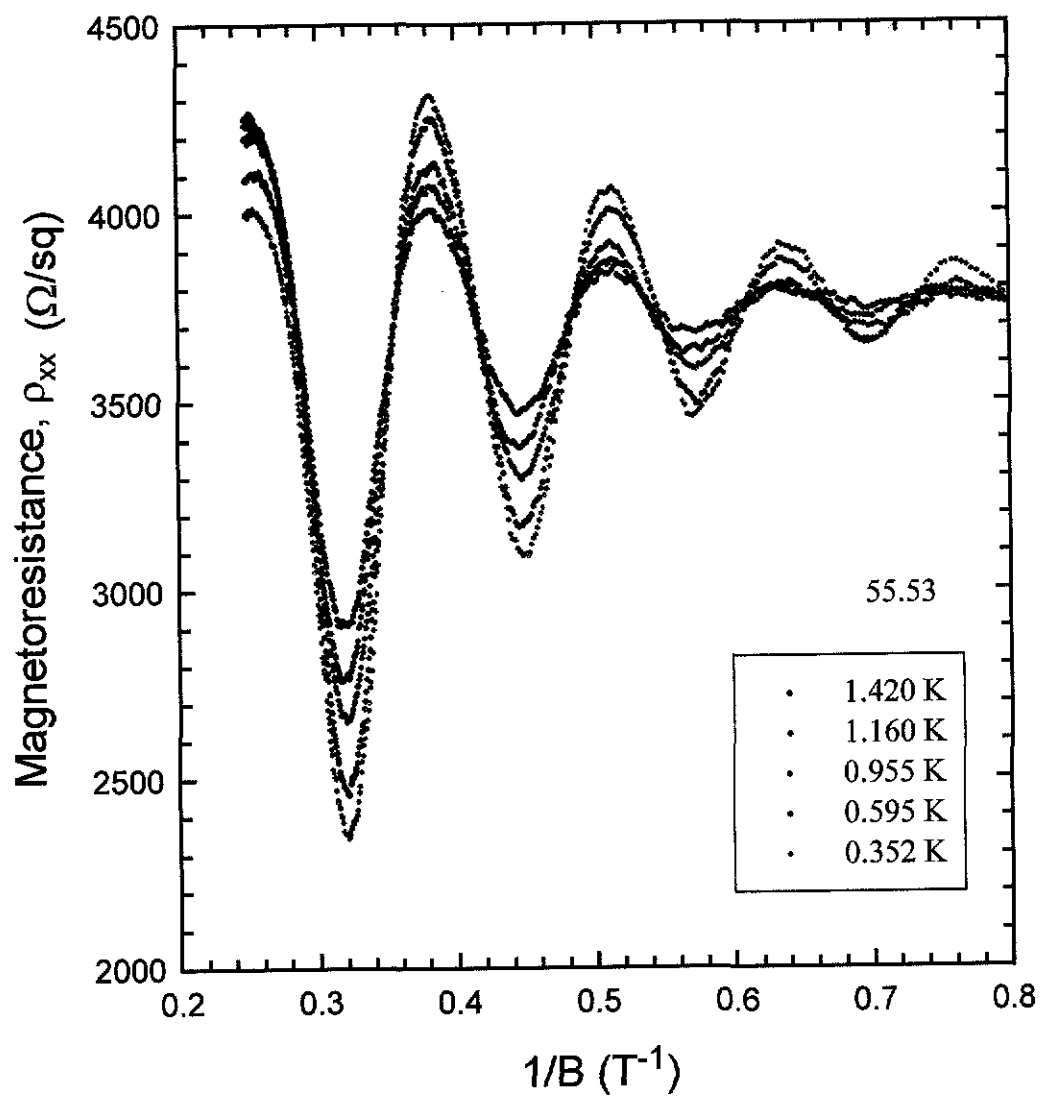


Figure 4.7: Shubnikov-de Haas oscillations of magnetoresistance as a function of $1/B$ for sample 55.51.

Magnetotransport measurements of the longitudinal sheet resistivity ρ_{xx} and Hall resistance ρ_{xy} were made in the range $B=-0.5-12$ T and $T=0.330-1.5$ K. The dependence of ρ_{xx} on B for various temperatures is shown in **Figure 4.6**. The shifts in positions of Shubnikov de Haas oscillation minima reflect the dependence of sheet density on B and the extracted values of 2DHG sheet density from the periodicity of ρ_{xx} vs $1/B$ plot in **Figure 4.7**, are in agreement with low field Hall measurements, indicating that only the first subband has been populated. At 0.3 K, Hall mobility is $4070 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$. From SdH low temperature magnetotransport measurements in the temperature range 332 mK – 2.5 K, the hole effective mass $m^*=(0.26\pm0.01)m_0$ was extracted for the corresponding carrier density of $n_s=3.8\times10^{11} \text{ cm}^{-2}$.

4.4 Lattice thermal conductivity results

The cryostat (shown in **Figure 3.7**) was designed, built and tested “in house” on a few standard samples before commencing thermal conductivity and thermopower measurements on Si/SiGe structures. The details of measurements were given in Chapter 3. The transfer of “heat” and the thermal isolation are essential considerations when designing a low temperature apparatus. The linear heat flow method has been used for thermal conductivity measurements. The experiments were carried out with a vacuum of 1.4×10^{-6} mbar and with a careful radiation shielding design.

In each low temperature apparatus one needs wires to carry signals from room temperature to the low temperature part, and back. For low current leads thin manganin ($\rho_{300K}=48 \mu\Omega\text{-cm}$, ($\rho_{4K}=43 \mu\Omega\text{-cm}$) wires have been used because of their low thermal conductivity and small temperature dependence of their electrical resistivity. During the thermal conductivity measurements, different top heater current values were used over the temperature range of 0.5-1.5 K (sample 31.17) and 1.5-300 K. **Figures 4.8 (a) and 4.9 (a)** show temperature difference dependence of the top heater current at 2.9 K and 4.6 K for the modulation doped 2DHG sample 31.17 and at 82.5 K for sample 32.12 (**Figure 4.10 (a)**). Temperature versus power of the top heater (RI^2) are shown in **Figure 4.8-10 (b)** for the same temperatures as in figures (a). R is a 120 Ω -strain gauge resistance used as a top heater attached to the sample. These figures show that ΔT is proportional to the applied power of the top heater. These are basic measurements and show the basic linear heat flow technique to be working correctly. If the sample is sufficiently isolated from its surroundings, any heat generated in the heater should go through the sample only and produce the appropriate temperature gradient. Another point is that the Joule heat generated should follow the law $Q=I^2R$. From these two assumptions the temperature gradient generated should have a square law dependency on the heater current. **Figures 4.8-10** show this to be so. Therefore heat is being correctly generated and transported through the sample.

Temperature dependence of thermal conductivity in the temperature range 1.5-300 K for three samples are shown in **Figure 4.11**. The data are close

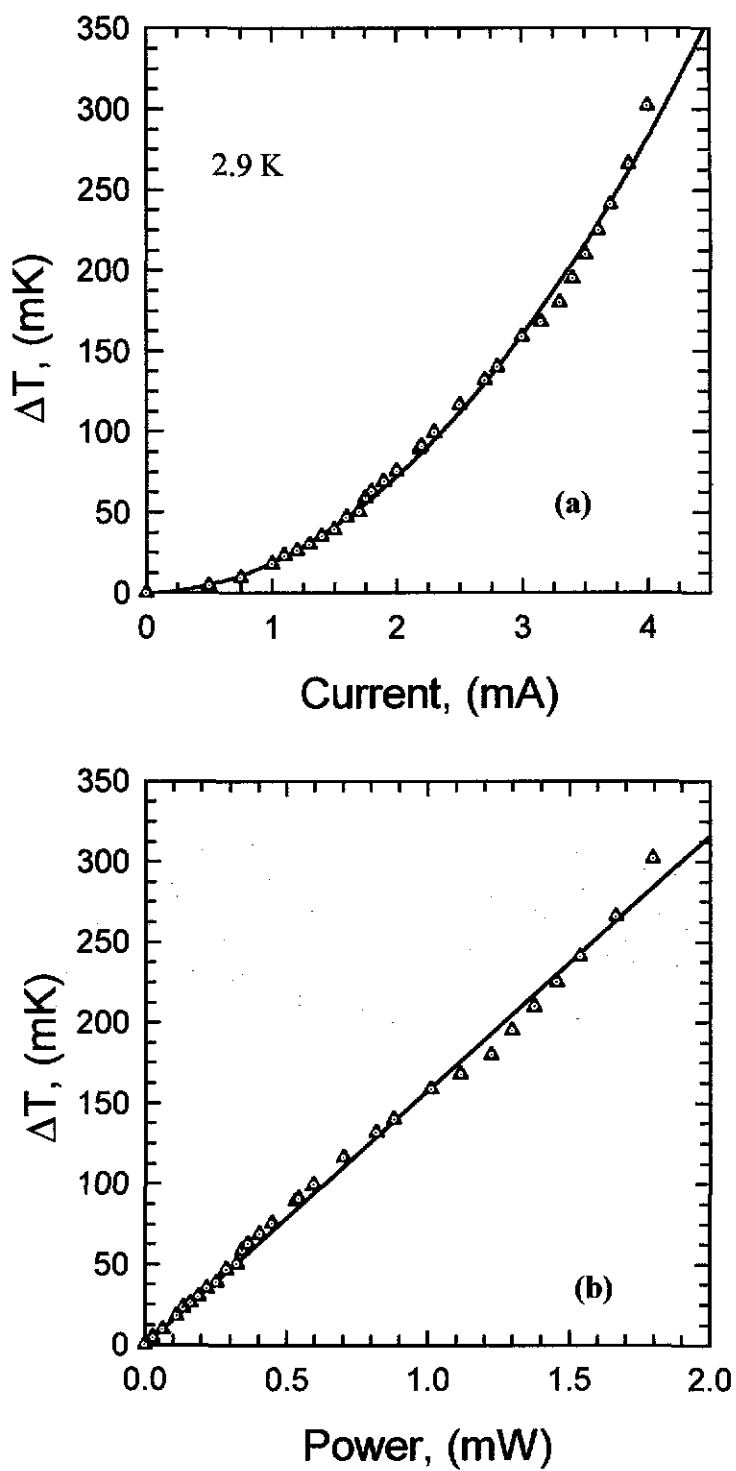


Figure 4.8: Temperature gradient dependence of heater current (a), and power (b) at 2.9 K for sample 31.17.

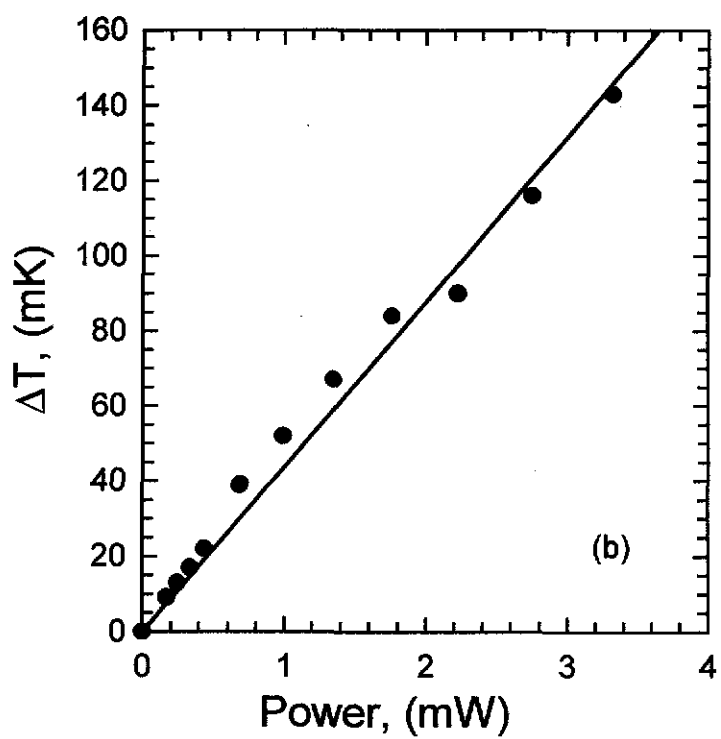
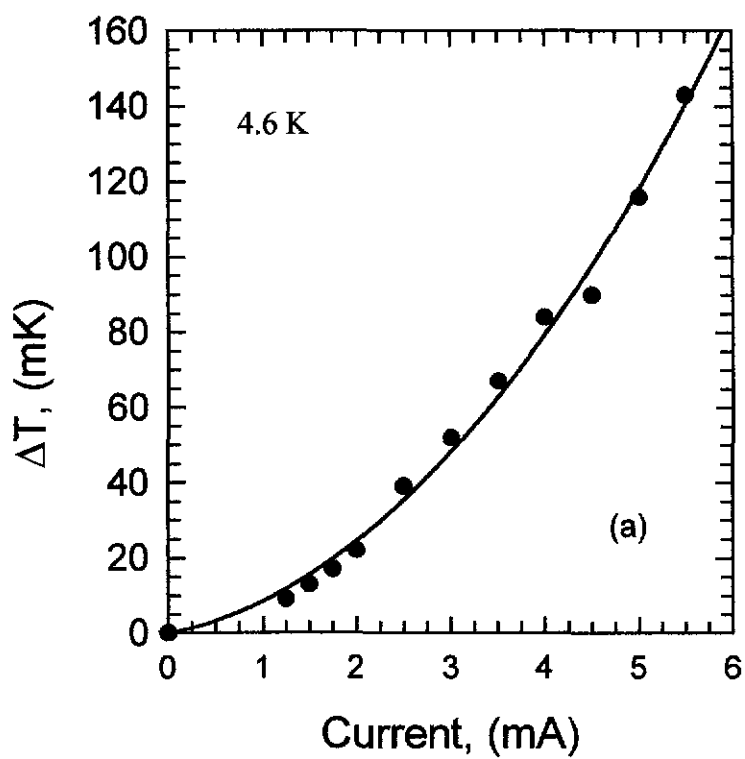


Figure 4.9: Temperature gradient dependence of heater current (a), and power (b) at 4.6 K for sample 31.17.

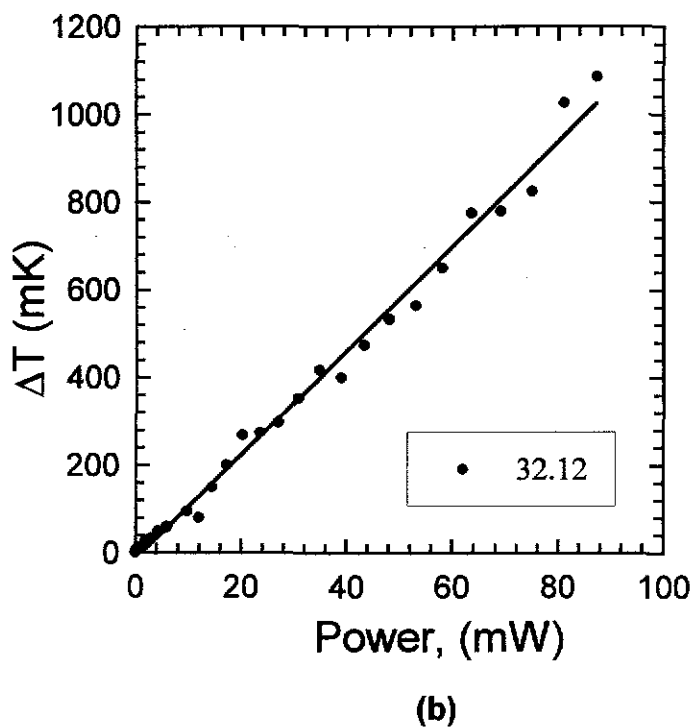
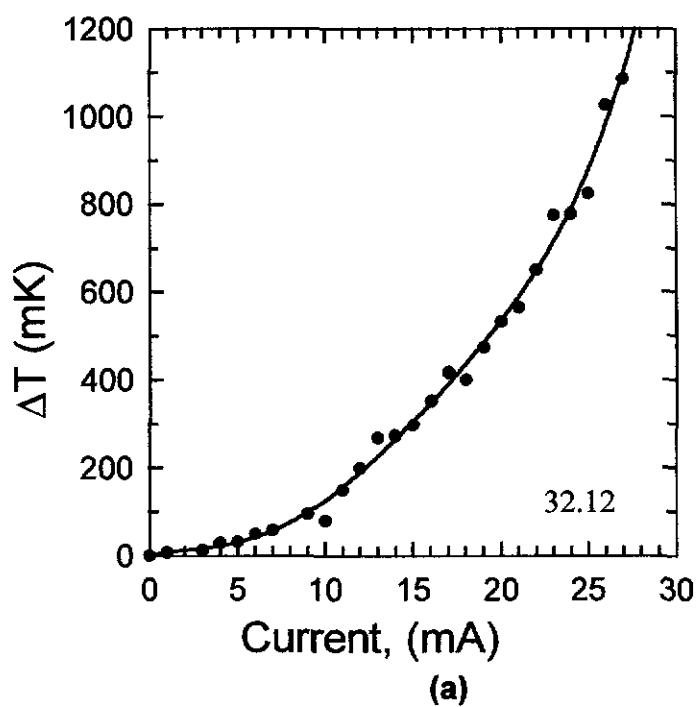


Figure 4.10: Temperature gradient dependence of applied heater current (a); and power (b) at 82.5 K liquid nitrogen temperature.

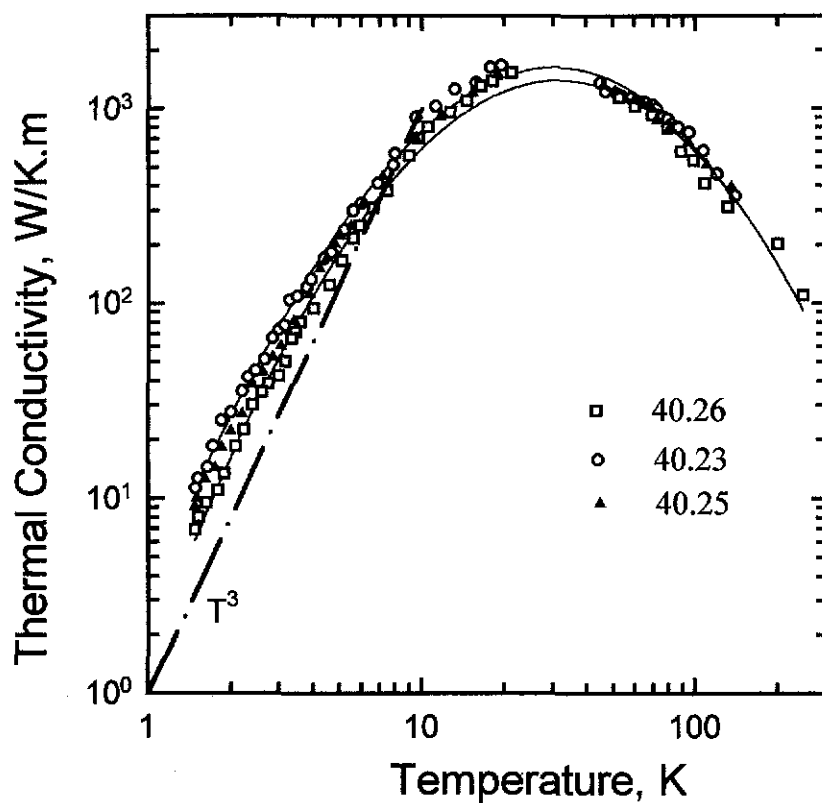


Figure 4.11: Thermal conductivity vs. temperature of five Si samples with different substrate doping concentrations (Solid lines are guide for eye). The dot-dashed line represents simply a T^3 , expected for pure boundary scattering.

to one another due to similar substrate doping levels: $n_s = 3.3 \times 10^{14} \text{ cm}^{-3}$, $4.4 \times 10^{14} \text{ cm}^{-3}$ and $3.25 \times 10^{14} \text{ cm}^{-3}$ at $T = 300 \text{ K}$ for samples 40.23, 40.25 and 40.26, respectively. We measure the thermal conductivity of the entire structure, substrate and strained SiGe alloy layer. **Figures 4.12 and 4.13** show a selection of results of thermal conductivity for the 2DHG samples in different composition to the substrate used for the heterostructures of this project. **Table 4.3** shows the doping levels and phonon mean free path of the substrates, as measured by the author. **Figure 4.14** shows temperature dependencies of thermal conductivity for 2DHG boron doped Si/Si_{0.87}Ge_{0.13} sample 31.17 and 2DEG Si sample 6B34G15. Sample 31.17 has been measured in the temperature range (0.5-1.5 K) (open circles) at the High Field Magnet Laboratory in Katholik Nijmegen University, the Netherlands. Two different measurements present the same thermal conductivity ($\lambda_L = AT^3$) curve using different types of calibrated temperature sensors and Si-diode. This curve is very accurate in terms of both measurements. Another sample (2DEG) which was created at a Si/SiGe heterointerface in the thin tensile strained Si layers were deposited on layers of unstrained SiGe alloy, using Si epitaxy, as shown in **Figure 4.14a**.

We show the thermal conductivity λ_L as a function of temperature for the samples. Near the maximum, around 20 K, thermal conductivity is particularly sensitive to sample imperfections and impurities. Boundary scattering should be dominant in our samples below 8 K. The value obtained for λ_L is thus close to that expected and accords well with the values obtained by Wybourne (1988). This correspondence, and the accurate T^3 dependence observed, is good

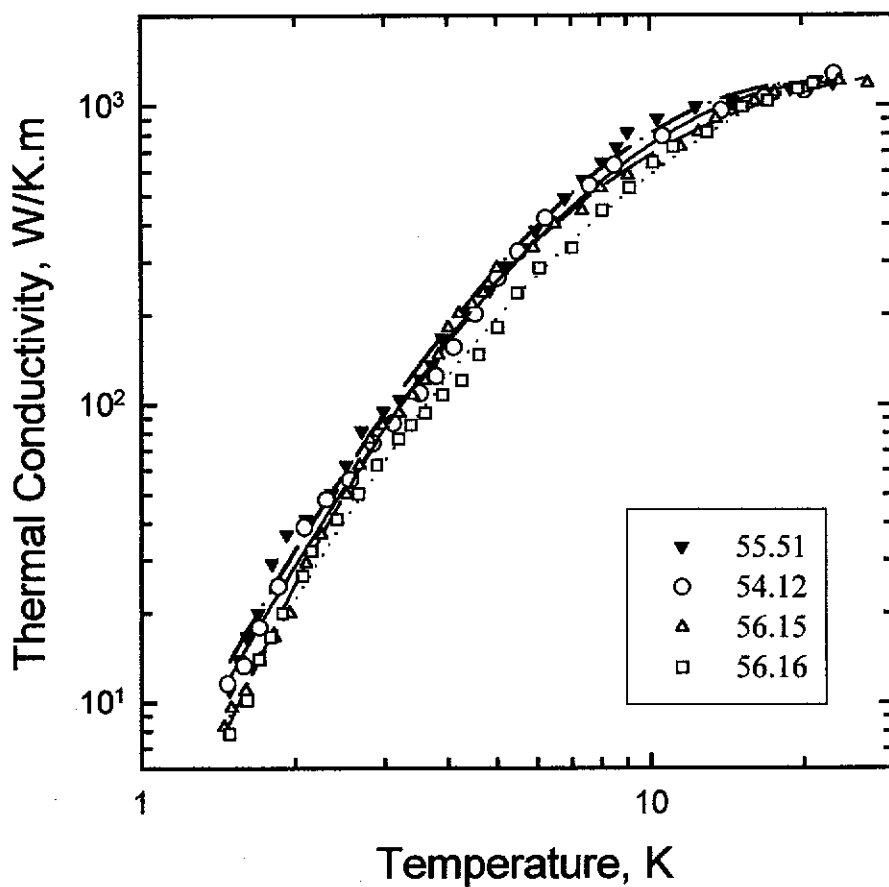


Figure 4.12: The measured thermal conductivities as a function of temperature with various substrate doping concentrations given in Table 4.3.

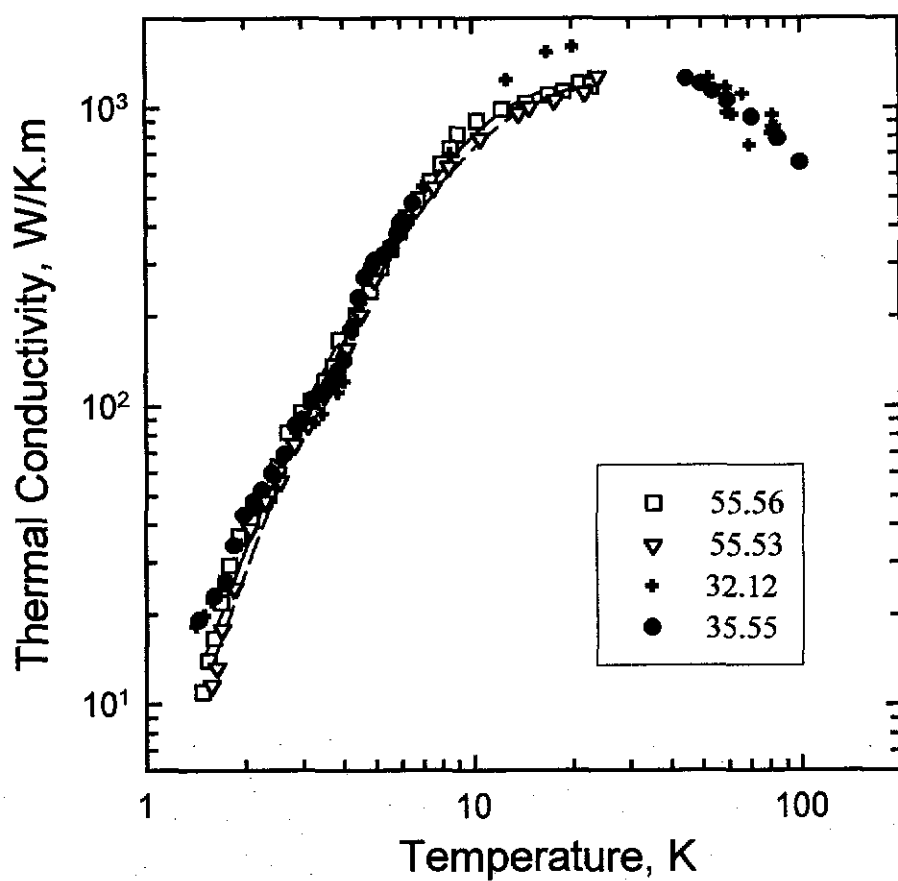


Figure 4.13: The measured thermal conductivities as a function of temperature with various substrate doping concentrations given in Table 4.3.

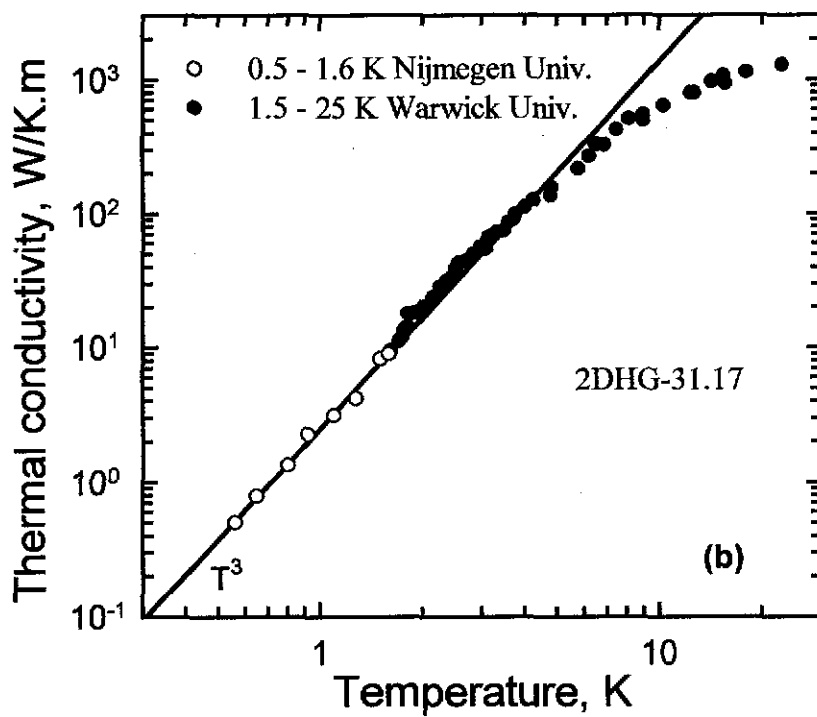
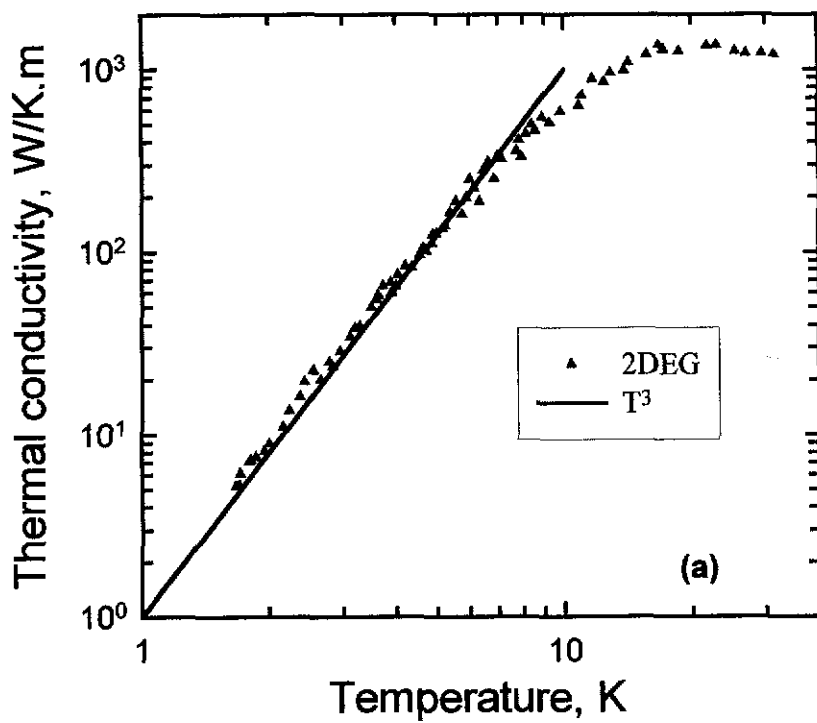


Figure 4.14: Variation of thermal conductivity with temperature for 2DEG (a) and 2DHG (b) samples. Solid line shows T^3 temperature dependence.

evidence that the method used for measuring the temperature difference was both accurate and precise.

Table 4.1: The physical structure of the samples. Here, letters are used as N (normal) and I (inverted) SiGe/Si 2DHG, E (epilayer) only Si:B samples.

Sample ID	Ge Conc.	L_{alloy} (nm)	L_{spacer} (nm)	L_{doping} (nm)	N_A 10^{18} cm^{-3}	m^*/m_e
31.17-N	0.13	30	20	50	2.5	0.28
31.18-N	0.12	30	20	50	2.5	0.28
32.12-N	0.05	30	20	50	4.0	0.23
35.55-N	0.29	20	20	30	2.5	0.29
40.21-N	0.19	22	10	50	4.0	0.29
40.22-N	0.19	22	4	50	4.0	0.31
40.23-N	0.20	22	2	50	4.0	0.38
40.25-N	0.18	22	45	50	4.0	0.30
40.26-N	0.20	22	60	50	4.0	0.31
47.07-E	---	---	---	25	3.0	---
47.74-N	0.07	40	8	50	2.5	0.25
50.36-E	---	---	---	25	2.0	---
54.12-N	0.20	20	12	50	2.0	0.27
55.51-I	0.23	17	20	30	2.0	0.24
55.53-I	0.17	17	20	30	2.0	0.26
55.56-I	0.20	17	20	30	2.0	0.26
56.15-N	0.20	17	6	30	2.0	0.25
56.16-I	0.20	17	14	30	2.2	0.25
Si 2DEG					5.0	0.19

The samples designated 40.21, 40.22, 40.23, 40.25 and 40.26 all have approximately the same germanium concentration (20%) and boron doping. The

only difference between them is the size of the undoped spacer layer. This set was designed to look at the effects of the sheet density variation in samples of the same germanium concentration.

Table 4.2: The physical structure of the samples and carrier density (n_s) and mobility (μ_H) values measured from Hall and van der Pauw measurements at 4.2 K.

Sample-ID	Ge conc.	$k_F \ell$	T_F (K)	ρ ($\Omega/\square$)	n_s (SdH) ($\times 10^{11} \text{ cm}^{-2}$)	μ ($\times 10^3 \text{ cm}^2/\text{Vs}$)
31.17-N	0.13	8.8	20	2610	2.0	1.11
31.18-N	0.12	8.8	20	2751	2.05	1.17
32.12-N	0.05			6917	0.97	1.16
35.55-N	0.29			13027	5.62	4.0
40.21-N	0.19				4.79	
40.22-N	0.19				7.65	2.3
40.23-N	0.20	6.2	90	3067	10.65	1.45
40.25-N	0.18			8489	2.07	2.75
40.26-N	0.20				4.6	1.48
47.74-N	0.07				8.0	8.0
50.36-E	---				4.5 (60 K)	0.20 (20 K)
54.12-N	0.20		52	2892	5.21	3.85
55.51-I	0.23		52	3620	5.05	3.39
55.53-I	0.17			4450	3.8	4.07
55.56-I	0.20		43		4.01	3.86
56.15-N	0.20	10.7	78		7.2	2.5
56.16-I	0.20				6.3	3.2
n-2DEG	---	335	33	50	4.5	260

Table 4.3: Relation amongst the substrate resistivity, doping concentration and phonon mean free path (pmfp).

Sample ID	substrate resistivity ($\Omega\text{-cm}$)	substrate doping concentration ($\times 10^{14} \text{ cm}^{-3}$)	pmfp, (mm) at 1.5 K
31.17	19.28	2.4	1.32
31.17	24.11	1.8	2.01
32.12	18.12	2.5	2.51
35.55	2.20	19.5	1.57
40.21	11.44	3.35	1.41
40.22	11.1	3.40	1.63
40.23	11.69	3.30	1.45
40.25	10.08	4.4	1.36
40.26	9.72	4.65	1.04
47.74	2.21	20	2.0
54.12	10.05	4.5	1.56
55.53	16.31	3.0	2.11

4.5 Phonon mean free path calculations

It is assumed that the electronic properties of the samples are affected by the phonon characteristics, and in particular the phonon drag thermopower is expected to vary linearly with the phonon mean free path. Experimental thermal conductivity (λ_L) data have been used to calculate the phonon mean free path (l_p) according to:

$$\lambda_L = \frac{1}{3} C_v l_p v_s, \text{ with } \frac{1}{v_s^3} = \frac{1}{3} \left(\frac{1}{v_t^3} + \frac{2}{v_l^3} \right) \quad (4-1)$$

where v_s^{-3} is the average inverse cube of the speed of sound for the three acoustic modes, $v_t = 5.331 \times 10^3 \text{ m s}^{-1}$, and $v_l = 8.861 \times 10^3 \text{ m s}^{-1}$ are the acoustic transverse and longitudinal modes in (001) Si at $T=80 \text{ K}$, respectively, we estimate $v_s = 5.896 \times 10^3 \text{ m s}^{-1}$ (Fletcher *et al.*, 1997). The result of our calculations is that C_v does not depend on Θ_D (Debye temperature) at the low temperature range because $T \ll \Theta_D$. The phonon mean free paths in the temperature range 1.5-250 K calculated from the experimental data for λ_L , are shown in **Figures 4.15 and 4.16**. **Figure 4.17** illustrates the phonon mean free path calculations for the 2DEG sample grown by UHV-CVD system (a) and down to 0.5 K temperature results are given for 2DHG MBE sample in (b).

In order to compare experimental data with theoretical phonon-drag calculations, we need the phonon mean free path l_p . The 2DHG plays an insignificant part in the magnitude of λ_L , which is completely dominated by phonons. At the lowest temperatures, l_p is determined by the boundaries. The phonon mean free path is strongly affected by the impurity concentration of the sample substrates (**Figure 4.18**). It is clear that the measured thermal conductivity is independent of the epilayer grown on the substrate, as no dependence on any epilayer characteristic could be found in the data. This is as would be expected. Aside from the intentionally varied surface characteristics and sample dimensions, the only significant differences between the samples is assumed to be the doping concentration in the substrate. Neither C_v nor v_s are

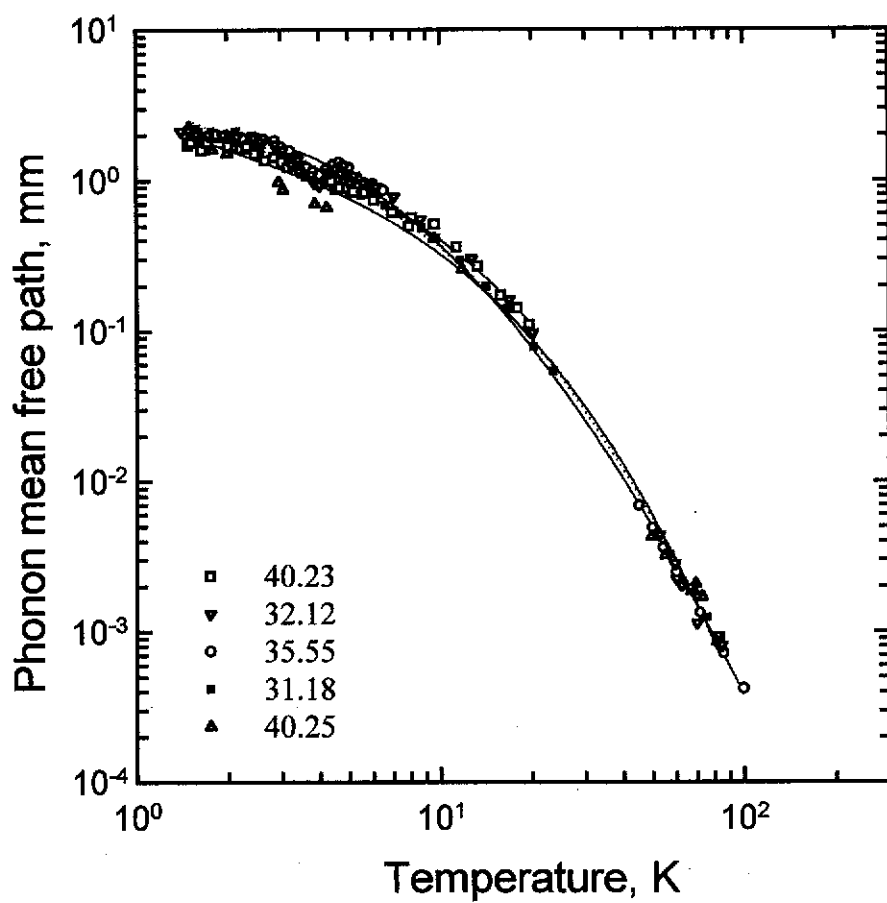


Figure 4.15: Phonon mean free paths extracted from measured thermal conductivity data.

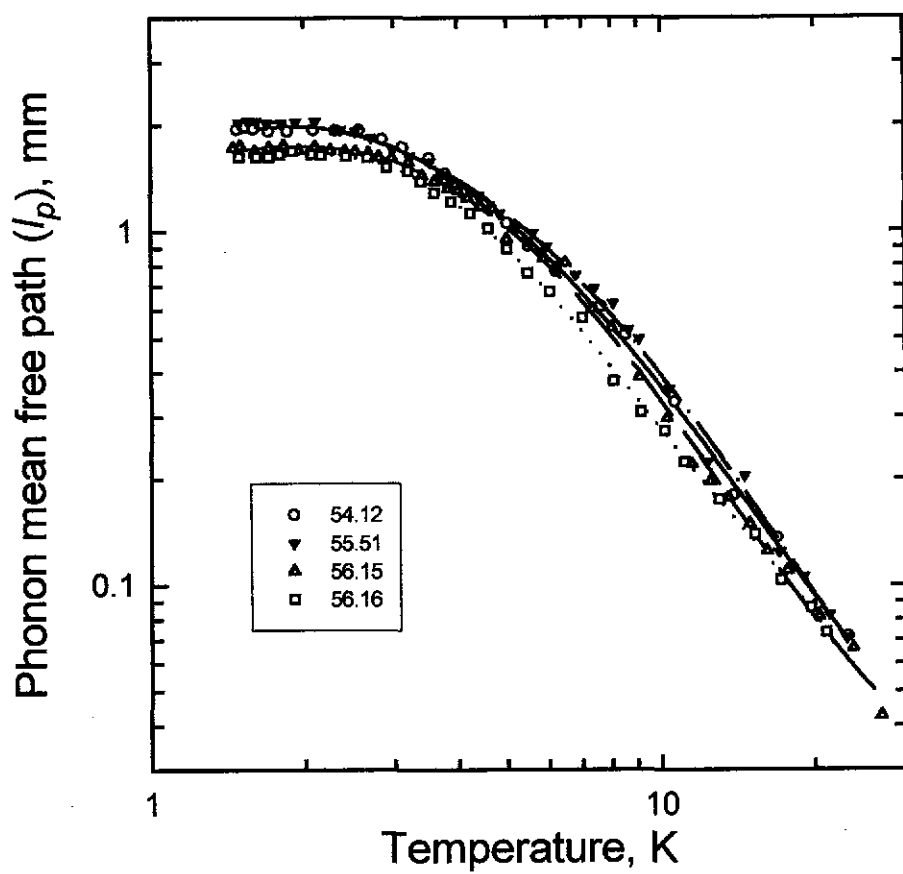
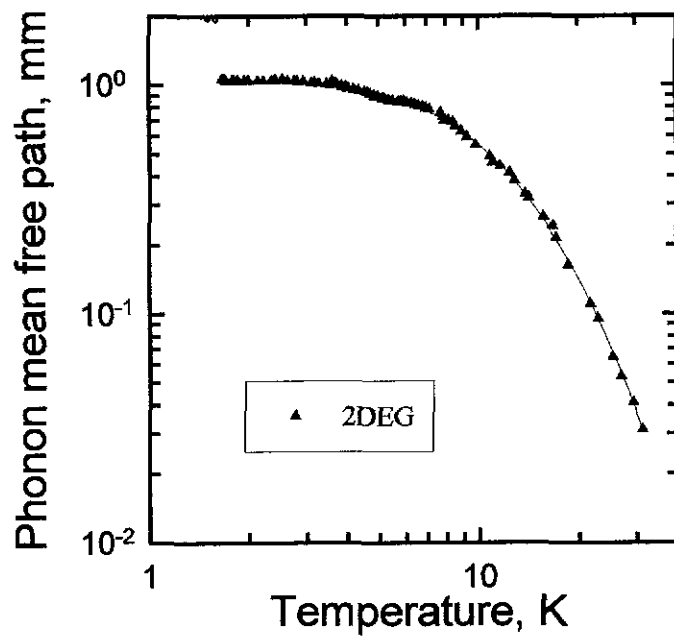
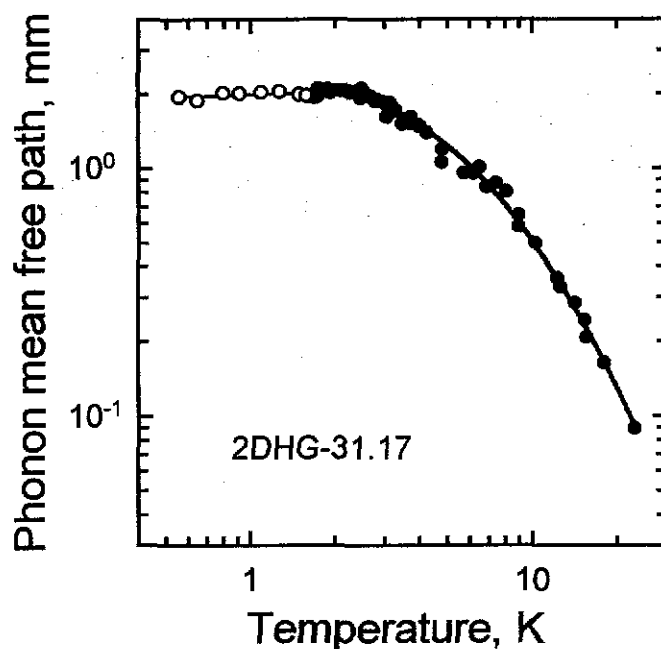


Figure 4.16: Phonon mean free paths calculated from thermal conductivity assuming $C_v \propto T^3$.



(a)



(b)

Figure 4.17: Phonon mean free paths as a function of temperature for 2DEG and 2DHG samples.

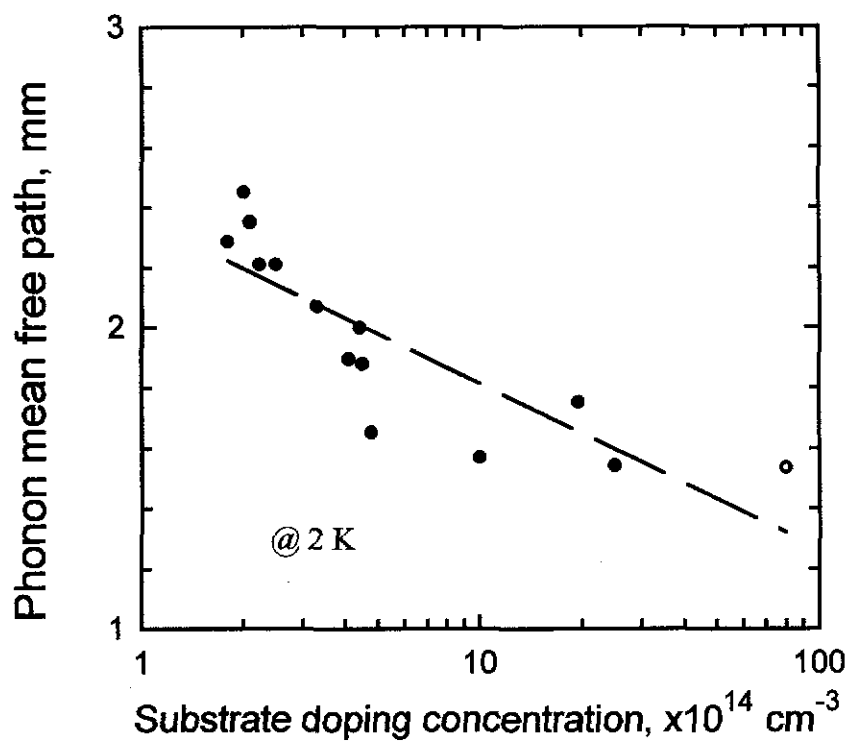


Figure 4.18: The phonon mean free path is affected by the impurity concentration of the sample substrates at low temperatures. Open circle shows high substrate doping concentration sample for delta doped layers (given in Chapter 5).

expected to vary significantly due to the impurity concentration in the substrate. This leaves I_p to be determined solely by the thermal conductivity measurements.

4.6 Thermopower measurements

In the last few years a great amount of experimental and theoretical research has been carried out on the thermoelectric properties of the two-dimensional electron (Cantrell and Butcher, (1987a, b); Ziannia, Butcher and Kearney, (1994); Fletcher *et al.*, (1994) and (1997), Tsaousidou *et al.*, 2000) and hole (Mironov *et al.*, 1997) gases in several semiconductor structures. A recent review on this topic, which is a continuation of an earlier review by Gallagher and Butcher (Gallagher and Butcher, 1992), has been published recently by Fletcher (1999). The thermopower is defined by $E=S\nabla T$, where E is the electric field and ∇T is the temperature gradient. There are two contributions to the thermopower observed: diffusion and phonon-drag. The first is due to the diffusion of carriers in the presence of a ∇T . The phonon-drag thermopower is due to the transfer of momentum from the non-equilibrium acoustic phonons to the carriers through the electron-phonon (or hole-phonon) coupling.

The temperature dependence of thermopower could thus be measured by variation of the heater current. The method usually gave agreement to within $\sim 10\%$, which is as an indication that the thermopower is linear ($\Delta V=S \Delta T$), and that possible systematic errors were small. Such errors would include temperature sensors and diode calibrations, possible thermal shorting or extraneous heating (the same amount of thermal offset would affect the results in

different proportions), and errors in zeroing the voltmeters. The zeroing is affected by waiting for the system to reach thermal equilibrium at the beginning of each run, while the heater is still off. The Si/SiGe heterostructure was grown by a solid source molecular beam epitaxy on a low doped (n-type, $1-25 \text{ } \Omega\text{-cm}$) Si (100) substrate. For one of these samples, the growth was started by 300-nm Si buffer layer, followed by a conduction channel consisting of a 30-nm strained $\text{Si}_{0.87}\text{Ge}_{13}$ layer followed by a 20-nm spacer and capped by a 50 nm Si-B doped layer at $2 \times 10^{18} \text{ cm}^{-3}$. The structure of sample and the valence band edge profile is shown in **Figure 4.19(a)**. Four strips contacts to the 2DHG were made by sputtering Al and annealing in nitrogen ambient at 490 °C for 45 minutes. **Figure 4.19(b)** shows the sample sizes and Al contacts for thermopower and SdH measurements. Contact resistance measurements are given in **Figure 4.19(c)**. More contact are has less resistance and also Au (Sb 1%) contacts of 2DEG sample have very low resistance (100 Ω /per contact) with comparing Al (Si 1%) contacts.

Using the experimental set-up described Chapter 3.5.6, the thermopower voltage ΔV between Al contacts was measured as a function of heater power. This varies the thermal difference between the contacts ΔT as well as the mean temperature T_m of the sample. The basic principle behind the measurement of the thermoelectric power is to apply a temperature gradient to a device and to measure the resulting voltage. Thermopower measurements require large enough temperature gradient so that a temperature interval ∇T can be produced across the sample. The results of the voltage difference vs. temperature difference were

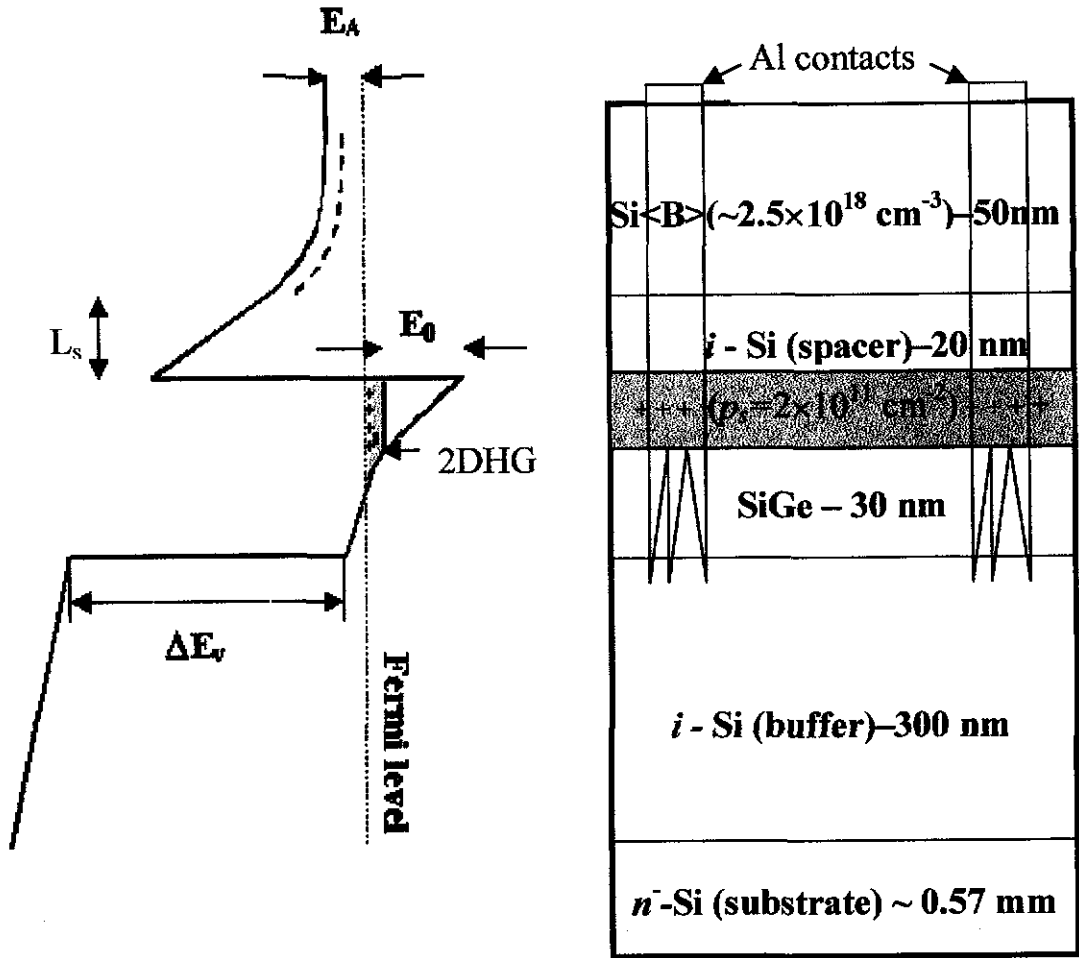
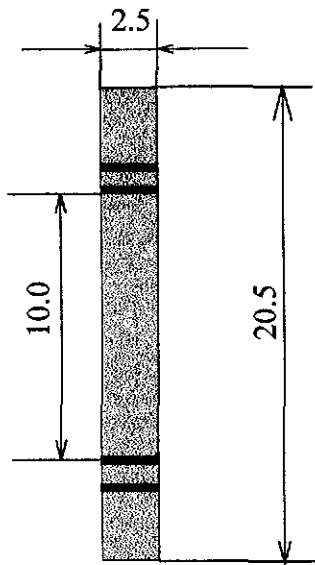
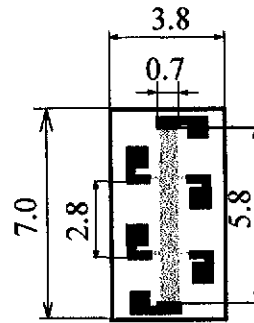


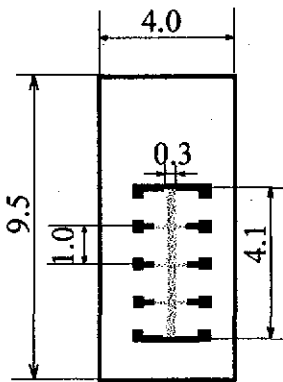
Figure 4.19(a): An example of a normally doped Si/SiGe/Si 2DHG structure and the valence band edge profile. E_A is the boron activation energy in Si, E_0 the lowest lying 2DHG energy level, L_s the dopant set-back distance and ΔE_v is the valence band offset energy.



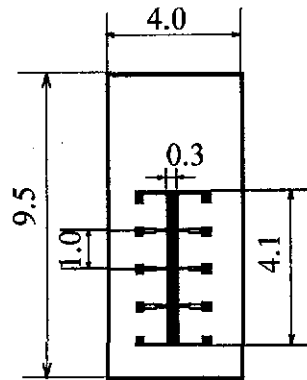
(1)



(2)



(3)



(4)

-  Mesa
-  Al contacts+ Mesa
-  Si substrate

Figure 4.19(b): Samples optimized for SdH (2) and thermopower measurements (1, 3 and 4) in.

All sizes are given in mm scale.

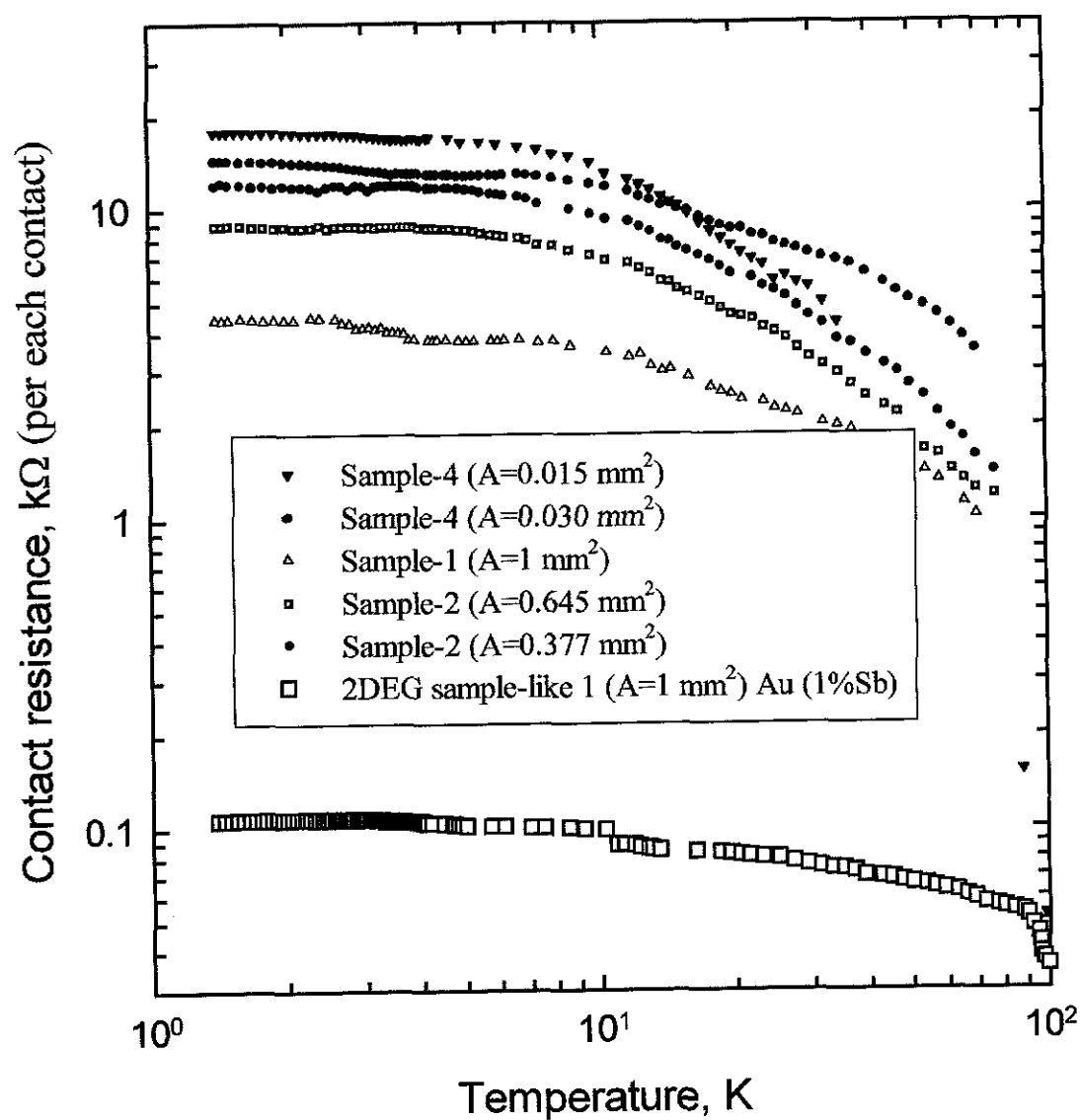


Figure 4.19c: Contact resistance dependence on temperature for sample shapes given in 4.19b. Au (1%Sb) contact area of the 2DEG sample was the same as Al (1%Si) contact area of the 2DHG sample given in (1). A gives contact area.

obtained at 2.9 K (**Figure 4.20a**) and 4.6 K (**b**) for sample 31.17 and voltage ($\Delta V + V_{\text{offset}}$) vs. temperature difference (**c**) were obtained for the sample 32.12 at 82.5 K. V_{offset} is zeroing voltage when the heater is off.

Measurements on thermoelectric transport in $\text{Si}/\text{Si}_{1-x}\text{Ge}_x$ heterostructures are presented for the first time. Several modulation doped $\text{Si}/\text{Si}_{1-x}\text{Ge}_x$ heterojunctions were measured with sheet carrier densities in the range 0.8 to $15 \times 10^{11} \text{cm}^{-2}$. The germanium content was from $x=0.07$ to 0.30 and the mobilities between 970 and $11100 \text{ cm}^2/\text{V.s}$. The results can be seen in **Figure 4.21**, the thermopower peaks at approximately $20\text{-}25 \text{ K}$. On the other hand, the theoretical thermopower reaches a maximum at 12 K and falls rapidly above this temperature, leading to an order of magnitude smaller than the experimental value at $T=25 \text{ K}$. Thermoelectric power results were obtained for all the same Ge composition (20%), both the normal and the inverted samples, in the temperature range $1.5\text{-}25 \text{ K}$ as shown in **Figure 4.22**. The behaviour appears roughly to be T^3 like below 5 K . Only a single subband is occupied in each sample. All data were taken by dc methods. The measured samples have sheet densities in the range of $(4.7\text{-}7) \times 10^{11} \text{ cm}^{-2}$ and the mobilities are in the range of $(3500\text{-}5000) \text{ cm}^2/\text{V.s}$.

The diffusion thermopower reflects the energy dependence of the relaxation time, and is determined not only by the magnitude of the scattering but also by details concerning the distribution of the scatterers and their type. The phonon drag thermopower involves the carrier-phonon interaction. The experimental data showed that the thermopower was proportional to the

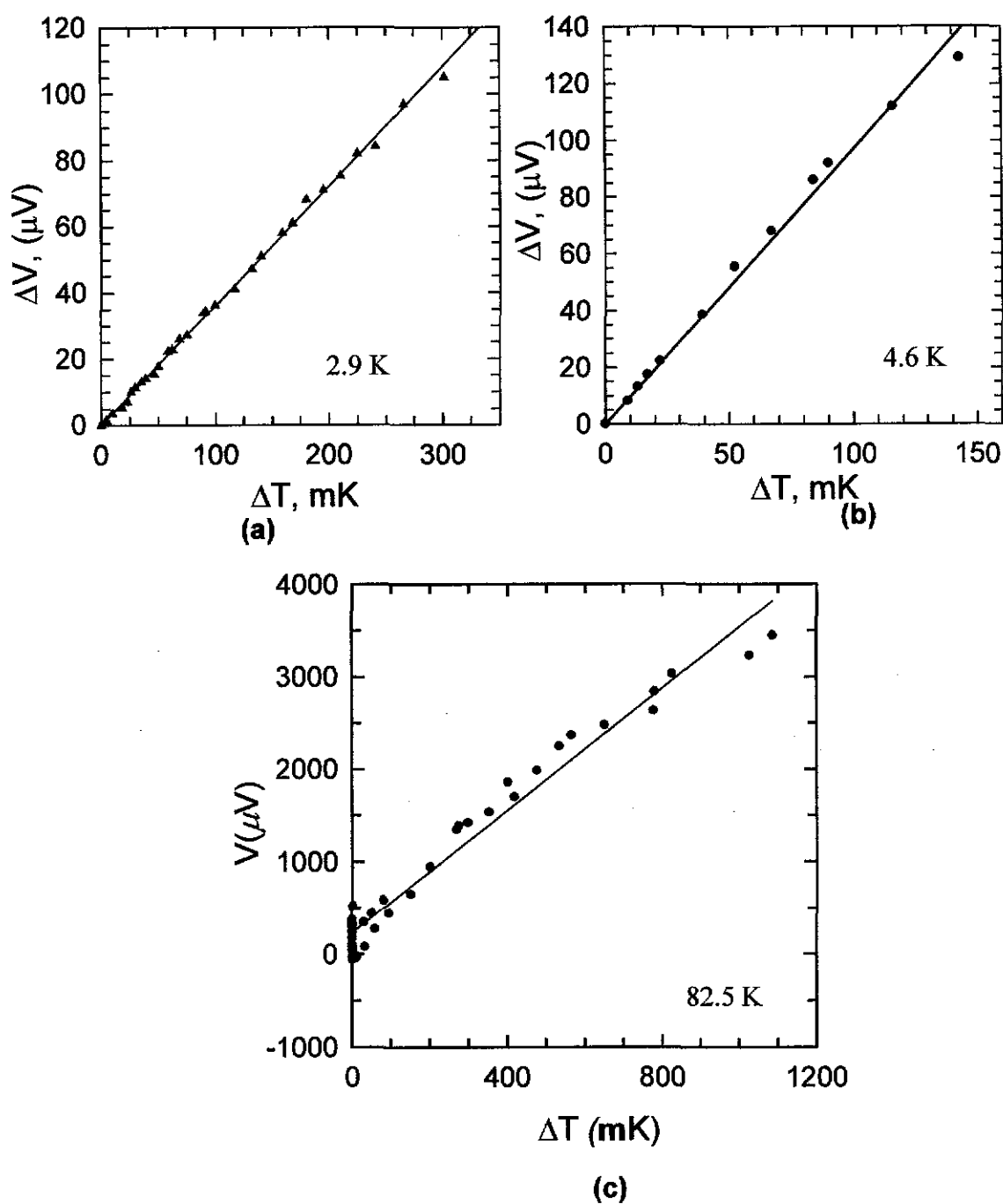


Figure 4.20: Thermopower voltage signal dependence on temperature difference (a) at 2.9 K and (b) 4.6 K for sample 31.17, and (c) voltage ($\Delta V + V_{\text{offset}}$) versus temperature difference at 82.5 K for sample 32.12.

V_{offset} is zeroing voltage when heater is off.

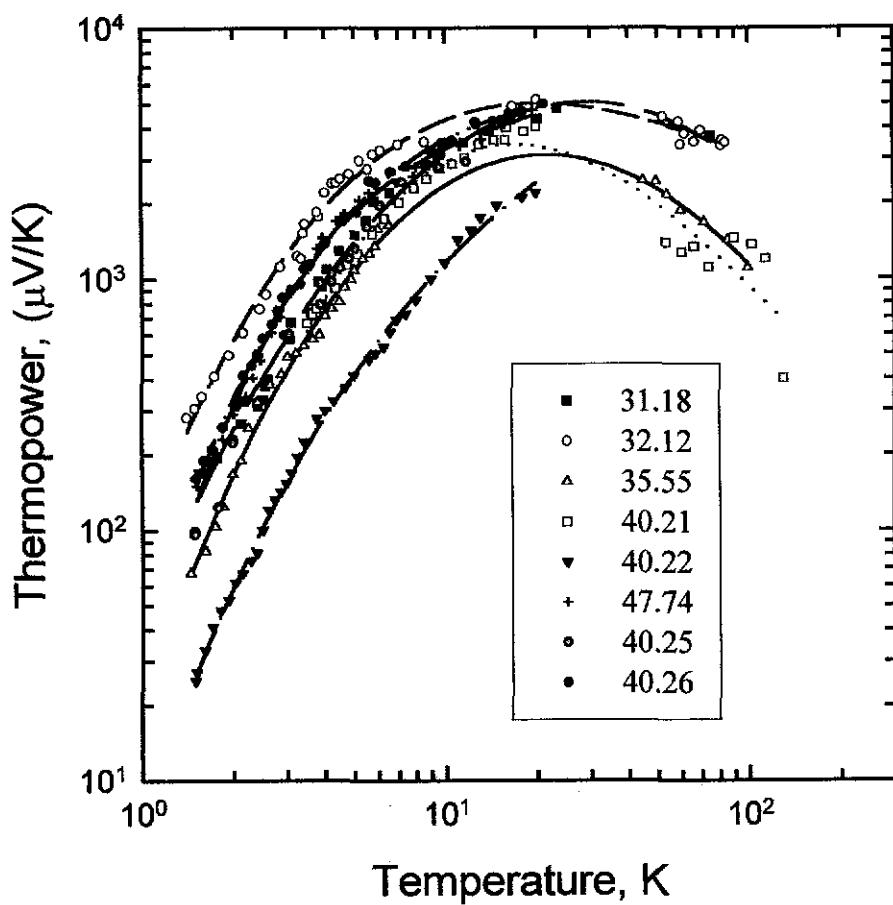


Figure 4.21: Temperature dependence of thermopower for various sheet carrier densities and germanium compositions of Si/Si_{1-x}Ge_x 2DHGs. The parameters are given in Table 4.1-3. The lines guide for eye.

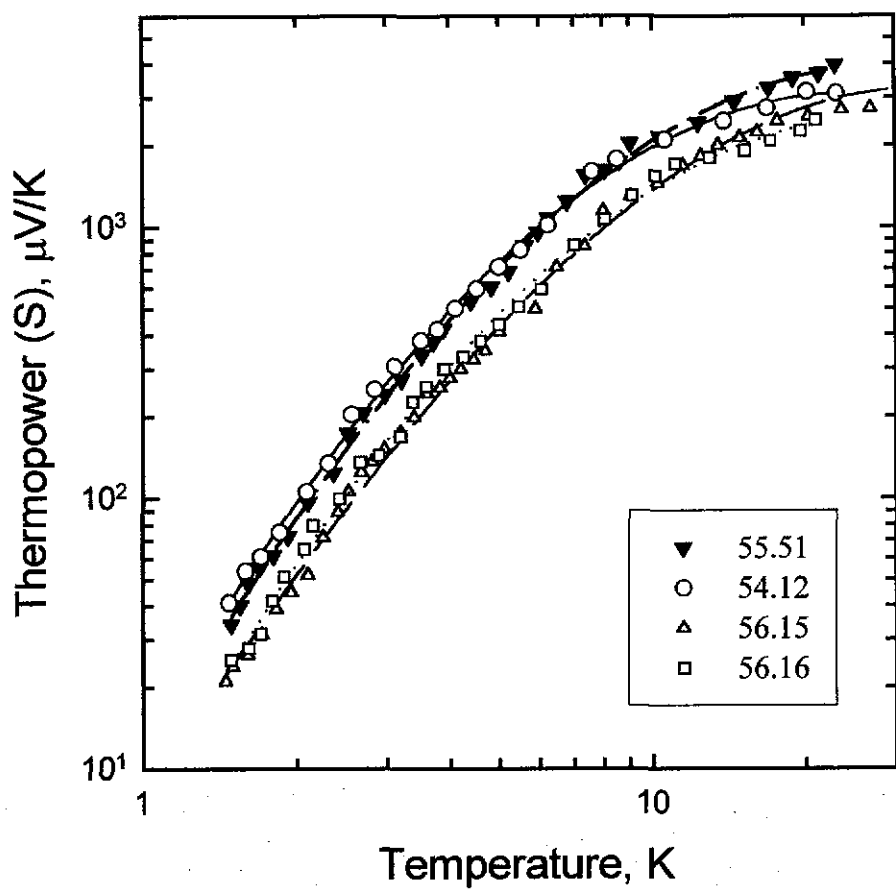


Figure 4.22: Temperature dependent on thermopower for normal and inverted doped 2DHG samples with various sheet carrier densities.

temperature cubed (T^3) below 10 K and was inversely proportional to the sheet carrier density. The data are now discussed by comparing them with diffusion and phonon drag thermopower theories.

4.6.1 Diffusion thermopower

The temperature gradient ∇T causes a diffusion of charge carriers which results in a charge separation producing an electric field. The charge flow stops once the electromotive force balances the thermal force. As a result, a contribution to the thermopower is due to the diffusion of charges, which is called diffusion thermopower.

Figure 4.23 shows the results for sample 31.17, with a theoretical phonon-drag thermopower fit to the data generated by M.Tsaousidou and P.N. Butcher using Cantrell-Butcher theory. Si/Si_{0.87}Ge_{0.13} 2DHG heterostructure sample has a $2 \times 10^{11} \text{ cm}^{-2}$ with $1.1 \times 10^4 \text{ cm}^2/\text{V.s}$ high mobility. The phonon mean free paths are as in **Figure 4.17 (b)**. Other data required for the calculations are the in-plane effective mass, m_p^* , taken from the data of Shubnikov de Haas, as reported by Whall *et al.*, (1995). The depletion layer concentration were taken as $N_{\text{dep}} = 1 \times 10^{11} \text{ cm}^{-2}$ for this and the other samples referred to below. The best fit for the data was obtained by taking an acoustic deformation potential, Ξ_{eff} of $(5 \pm 0.5) \text{ eV}$. The diffusion thermopower is supposed to be linear in temperature (Eq. 2-14) and one can therefore write $S_d = AT$ where A is a constant. The diffusion component to the thermopower for this sample may be estimated as $S_d = 12T \text{ } \mu\text{V/K}$. This is plotted as the straight line in

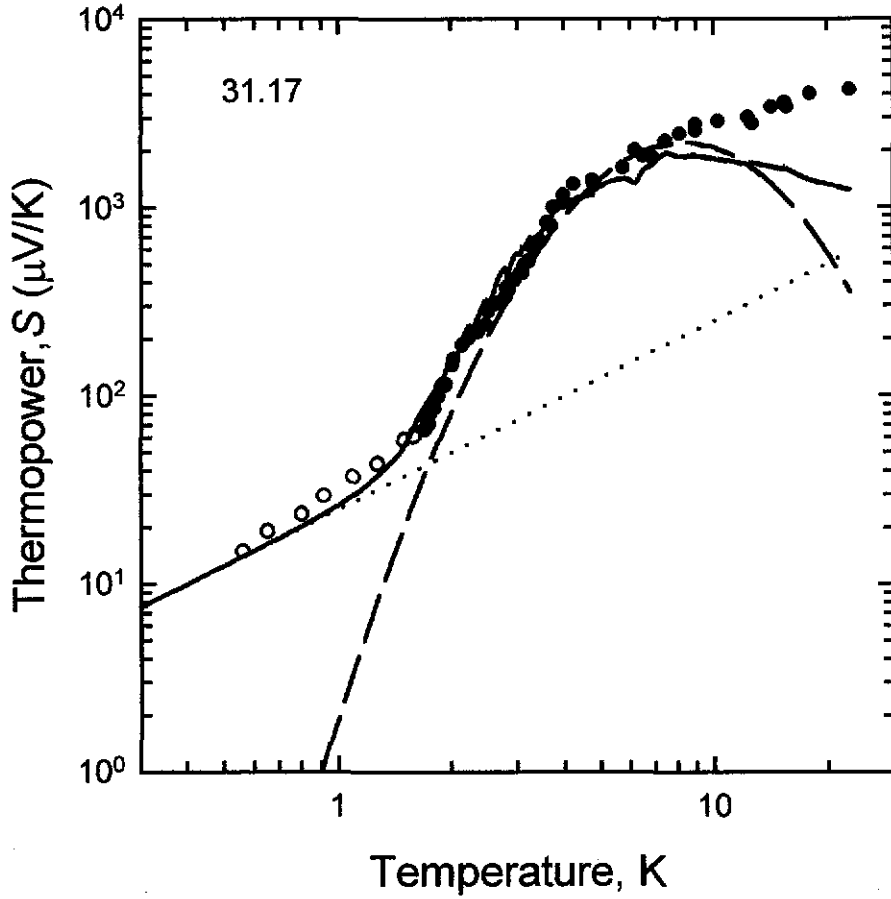


Figure 4.23: The thermopower, S , as a function of temperature. The open circles and full circles are the experimental data in the temperature ranges 0.5 – 1.6 K and 1.5 – 25 K, respectively. The broken line is the theoretical estimation of S_g by using $\Xi = 5$ eV as are explain in text. The dots are the theoretical values of S_d with $p=1$. The total thermopower calculation is shown by the solid line. Si/Si_{0.87}Ge_{0.13} 2DHG heterostructure sample has $2 \times 10^{11} \text{ cm}^{-2}$ with $1.1 \times 10^4 \text{ cm}^2/\text{V.s}$ high mobility.

Figure 4.23 along with the phonon-drag and diffusion combined, and experimental results for 31.17. The combined results for diffusion and phonon drag produce a qualitative fit for the data for sample 31.17 which seems to reproduce the appropriate characteristics of a 2D system as shown by Fletcher and co-workers previously (Fletcher *et al.*, 1994, Cyca, Fletcher and D'Iorio, 1992). Calculations of the phonon-drag thermopower (solid line) according to Eq. (2-15) correspond well with the experimental results in the temperature range 1.0-10 K. The only adjustable parameter in this calculation is the coupling constant (5 ± 0.5) eV. The in-plane effective mass m^* has been taken from temperature dependent SdH data and those in the growth direction have been assumed to be given by $m_t^* = 1.36 m^* (k=0)$ (Chun and Wang, 1992) and is $m^* = (0.24 \pm 0.01) m_0$. Fermi energy (E_F) is 1.8-2.0 meV and Fermi temperature is $T_F = 21-23$ K. The experimental thermopower in the zero magnetic field S , is temperature dependent approaching $S \propto T^3$ between 2.5 and 5 K, and $\propto T^4$ 1.5 - 2.5 K in the temperature range (Agan *et al.*, 2000a).

In Mott's equation (Eq.2-14), the parameter p is determined by the energy dependence of the transport lifetime τ . The parameter p is a function of sheet carrier density, n_s , and its magnitude is of the order of the unity depending on the scattering mechanism (background impurities scattering $p = -2.95$, interface roughness scattering $p = 1 - 1.2$, remote impurities scattering $p = 1.2-1.5$), as calculated by Karavolas *et al.*, (1990). It has been observed experimentally that $S_d \sim T$ (diffusion thermopower only) could be observed at $T < 1.5$ K and for the sheet carrier density $n_s = 2 \times 10^{11} \text{ cm}^{-2}$ for $\text{Si}_{0.87}\text{Ge}_{0.13}$ /Si (100) quantum-well

(31.17). p is approximately 1. This is the closest to the theoretical calculation for remote impurity scattering.

To reach low temperatures (0.5-1.5 K) in the experiments on 2DHG (sample 31.17), the experiment was set up in a $^3\text{He}/^4\text{He}$ -dilution refrigerator at the High Field Magnet Laboratory in Katholik Nijmegen University, The Netherlands. Since the sample has to be in vacuum to ensure a uniform temperature gradient, a hysol sample holder was designed which placed the sample in the inner vacuum space underneath the mixing chamber.

A heater was glued with stycast epoxy directly to the other end of the sample. We used strain gauges as heater resistors. The heater and thermometers were connected to the contact board by 50 micron manganin wires to ensure that the applied heat was conducted to the cold sink through the sample only. The wiring was achieved using twisted pairs of 100 micron manganin wires. The wiring for the thermometers and heaters consisted of double twisted pairs which enabled 4-point measurements. The thermoelectric power of manganin, which has to be considered due to the temperature differences of the contacts, was negligible compared to the thermopower of the 2DHG. The bond wires were connected to the contact pads of the heterostructure with epo-tek, a silver filled epoxy that provides low resistance contacts with high mechanical strength. The thermoelectric power was measured as dc. measurements, which is mainly useful in a zero magnetic field using an analogue EM-Electronics nanovoltmeter. Data acquisition was automated by taking averages when turning the heater switch on and off many times. An accuracy of about 1 nV standard deviation was achieved

for the thermoelectric voltage. This small error enabled us to measure the zero field thermopower down to 250 mK where signals, typically, are as low as a few nanovolts.

The sample masks defining the Hall bar for the sample 31.17 were designed by the author for the specific requirements of the thermopower measurements in the Department of Physics, at Warwick University. The amplitude of the measured voltages depends on the applied temperature gradients. In contrast to resistivity measurements, where the applied current can be varied over a wide range, the range of applied gradients is much more restricted because a strong increase in heater power heats up the sample considerably. Therefore, signals at low temperatures are typically in the order of microvolts or less. In order to obtain the maximum temperature difference between contacts, the Hall bar has to be as long as possible (in our case the length of the mesa is $l_m=4.1$ mm). A typical sample of masks and mesa is shown in **Figure 4.19 (b) (3)**. Note that the measured voltage does not depend on the geometry factors l_m/w_m . The thermopower S is best measured on what would be called ‘current contacts’ in a resistivity measurement. Note that in a thermopower measurement there are no current contacts since the driving force for the potential difference is the temperature gradient.

For a typical thermopower measurement at $T=500$ mK, the temperature difference between the contacts is $\Delta T \cong 40$ mK. The experimental error in determining ΔT is about 2 mK giving a relative statistical error of 5%. The

accuracy of the absolute temperature is estimated to be 1%, which gives an error of 6% in the absolute value of thermopower.

4.6.2 Phonon drag thermopower

Figure 4.24 shows the thermopower results for sample 40.23. The sample 40.23 has a Fermi degeneracy temperature high enough for the 2DHG to fully degenerate through the entire modelled temperature range. The sample has the highest carrier density ($1.05 \times 10^{12} \text{ cm}^{-2}$) of Si/Si_{0.8}Ge_{0.2} 2DHGs and so offered the best chance of obtaining good high temperature results. An observation of the data now offers an insight into the qualitative aspects of these thermopower measurements. The expected value of the diffusion component S_d in this region was less than 20 $\mu\text{V/K}$. The inclusion of piezoelectric scattering in the calculations may improve correspondence with the data. The origin of the piezoelectric coupling was attributed to a strain induced change in the ionicity. Piezoelectric scattering is expected to become more significant as the lattice temperature is reduced. Good correspondence with the experiment is obtained only if scattering of the acoustic mode phonons by both the deformation potential and the piezoelectric coupling mechanisms are considered. The piezoelectric constant for coherently strained Si_{0.8}Ge_{0.2} is not known. But, we are able to deduce a value for the piezoelectric constant for Si_{0.8}Ge_{0.2} (Braithwaite *et al.*, 1997). The importance of such piezoelectric-like behaviour has been confirmed through direct measurements of the reversible electromagnetic wave to sound wave conversion in similar MBE grown Si/SiGe/ (001) Si

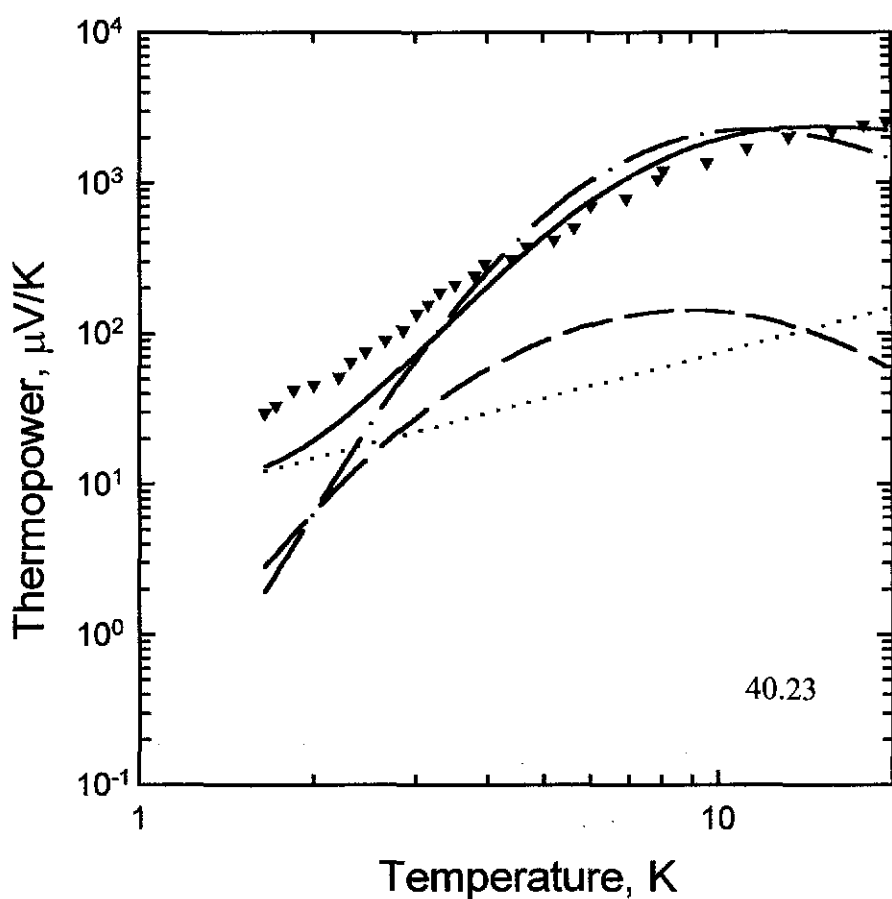


Figure 4.24: Thermopower as a function of temperature for the highest sheet carrier density ($1.05 \times 10^{12} \text{ cm}^{-2}$) of Si/Si_{0.8}Ge_{0.2} 2DHG sample. μ is 1450 $\text{cm}^2/\text{V.s}$. Triangles show measured thermopower. Dotted line is S_d ($p=1$), dashed-dotted line is S_g ($\Xi=4.5$ eV), dashed line is piezo-electric contribution ($h_{14}=0.5 \times 10^7$ V/cm) and solid line shows total estimated thermopower, S .

heterostructures (Khizhny *et al.*, 1996). In fact, the voltage offset at zero applied temperature gradient is (and typically) only 5 microvolts, which corresponds to approximately 5% of the voltage for typical measurement temperature differences (~ 50 mK). Noise is usually less than 0.5%. The pronounced discrepancy between experiment and theory at $T > 12$ K can be understood on the basis of (a) the different average phonon mean free paths involved in thermal conductivity and thermopower, (b) the loss of degeneracy of the 2D hole gas, and (c) the existence of 3D conduction through the doped cap layer parallel of the 2D hole gas in our heterostructures at $T > 20$ K. The dashed-dotted line in **Figure 4.24** shows the theoretical estimations of the phonon drag contribution S_g according to Eq. (2-15), including a piezoelectric interaction with the coupling constant $h_{14} = 0.5 \times 10^7$ V/cm (dashed line). The solid line gives the total thermopower calculations ($S_g + S_d + S_{piezo}$). The in-plane effective mass m^* has been taken from SdH data and those in the growth direction have been assumed to be given by $m_t^* = 1.36 m^*$. The sample has, $m^* = 0.38 m_0$ effective mass, 1.05×10^{12} cm $^{-2}$ sheet carrier density and 1440 cm ^{2} /Vs mobility at 4.2 K. Moreover, the hole wavefunctions in the direction of the confinement are described by the Fang-Howard variational functions and the value of the depletion is 10^{11} cm $^{-2}$. The detailed study of the hole-phonon interaction in strained Si/SiGe is very laborious because of the complicated band structure of Si and Ge and the phonon drag problem in 2DHGs. To make the calculations easier, we assume an isotropic energy band so that the hole phonon interaction is described by a single acoustic deformation potential Ξ_{eff} . For the sample 40.23 we found that the best

correspondence between the theoretical and experimental values of the thermopower, for temperatures up to ~ 12 K, occurs for $\Xi_{\text{eff}} = 4.5$ eV (screened hole-phonon interactions). We took $p=0$ due to the lack of adequate experimental information about this parameter at the moment. Moreover, when $k_B T < 0.1 E_F$, p does not affect the accuracy of the calculations. The Fermi temperature T_F is 92 K. It falls between the values for the two elements, $\Xi_{\text{Si}} = 7.9$ eV and $\Xi_{\text{Ge}} = 3.7$ eV reported by Wiley (1970). It also corresponds well with the values deduced recently from the hot carrier SdH measurements on the same structure (Brunthaler *et al.*, 1996).

To conclude, the thermopower of a 2DHG in Si/Si_{0.8}Ge_{0.2} has been measured for the first time and is found to be dominated by phonon drag in the temperature range 1.5-25 K. From the thermopower data, the deformation potential for acoustic phonon scattering was estimated to be 4.5 eV in strained Si_{0.8}Ge_{0.2}; a result with no other adjustable parameters. At temperatures between 1.5-4 K the experimental thermopower was significantly larger than that given by the phonon drag theory. Mironov *et al.*, (1997) have mentioned that this possibility could be accounted for by a piezoelectric scattering contribution to the phonon drag thermopower. The maxima of (2-3) mV/K near 20 K are caused by phonon drag.

Modulation doping was used to reduce carrier scattering moving to the doped region from the conduction channel region. Si/SiGe 2DEG was found to have high electron mobility at low temperatures and to have opened up the possibility of improving the room temperature performance of Si devices (Sadek

and Ismail, 1995). The 2DEG itself, is formed in a tensile strained Si layer grown on strain relaxed SiGe alloy layers. The tensile strain splits the sixfold degenerate conduction bands, making the four in-plane conduction band valleys rise in energy and the two growth direction valleys reduce in energy to form a quantum well. The relaxed SiGe layers have a larger lattice constant than Si, and are conventionally formed by growing a virtual substrate consisting of a thick alloy layer on a Si (001) substrate, which exceeds a critical thickness for strain relaxation.

The modulation doped 2DEG structure was grown in a cold-walled ultrahigh vacuum (UHV) compatible stainless steel chemical vapour deposition (CVD) system, using SiH_4 and GeH_4 with H_2 as a carrier gas in the Defence Evaluation and Research Agency, Electronic Sector, Great Malvern, UK. In the present study, the structure consisted of a graded SiGe alloy buffer grown on a Si (001) substrate followed by a buffer region of a constant Ge mole fraction ($x=0.25$) to form the virtual substrate, on which the channel regions were grown. The constant composition buffer was $\sim 0.8 \mu\text{m}$ in thickness, the grade region was $\sim 4 \mu\text{m}$. The modulation doped 2DEG layer consisted of an additional $\text{Si}_{0.75}\text{Ge}_{0.25}$ alloy buffer, a tensile strained Si layer of nominally 9 nm in thickness and a $\text{Si}_{0.75}\text{Ge}_{0.25}$ spacer region of 35 nm, followed by an As doped region of about 90 nm thickness and a thin Si cap layer. The device was optimised for low temperature electrical characterisation and parallel conduction in the substrate and doped regions at room temperature (Churchill *et al.*, (1997 and 1998)). The temperature dependence of the thermopower was measured from room

temperature down to 1.5 K in the Si 2DEG sample and in the Si/Si_{0.8}Ge_{0.2}/Si inverted modulation doped heterostructures grown by Molecular Beam Epitaxy (MBE). Comparisons were then made between the theory and the present results and other experimental works. The zero-field results were predicted by classical theory and depend upon electron concentration. **Figure 4.25 and 4.26** show the results of the experimental and theoretical work on three further samples that have been thoroughly characterised previously. The 2DEG (Si) sample has $4.5 \times 10^{11} \text{ cm}^{-2}$ sheet carrier density and a high mobility of $2.6 \times 10^5 \text{ cm}^2/\text{V.s}$. A $\Xi_a = 9 \text{ eV}$ and $\Xi_d = -6 \text{ eV}$ ($g_v=2$) deformation potential (screened deformation potential) has been used. The inverted sample 55.51 (2DHG) Si/Si_{0.8}Ge_{0.2} has a $4.7 \times 10^{11} \text{ cm}^{-2}$ sheet carrier density and a low mobility of $3.5 \times 10^3 \text{ cm}^2/\text{V.s}$. The normal doped (2DHG) Si/Si_{0.8}Ge_{0.2} has sheet carrier density of $7 \times 10^{11} \text{ cm}^{-2}$ and a low mobility of $2.5 \times 10^3 \text{ cm}^2/\text{V.s}$. Both 2DHGs samples were fitted using $\Xi=2.5 \text{ eV}$ unscreened hole-phonon interactions and 4.5 eV screened hole-phonon interactions phonon drag thermopower. This corresponded well with the 3 eV unscreened deformation potential that was carried out with hot carrier measurements on the same samples as in our group by Ansaripour *et al.*, (2000).

The present measurements promise new information regarding the relevant mobility that limit scattering mechanisms for device operation at room temperature. We have obtained experimental data for the thermopower in the temperature range 1-10 K, which shows phonon-drag thermopower temperature dependence in accordance with Cantrell-Butcher theory.

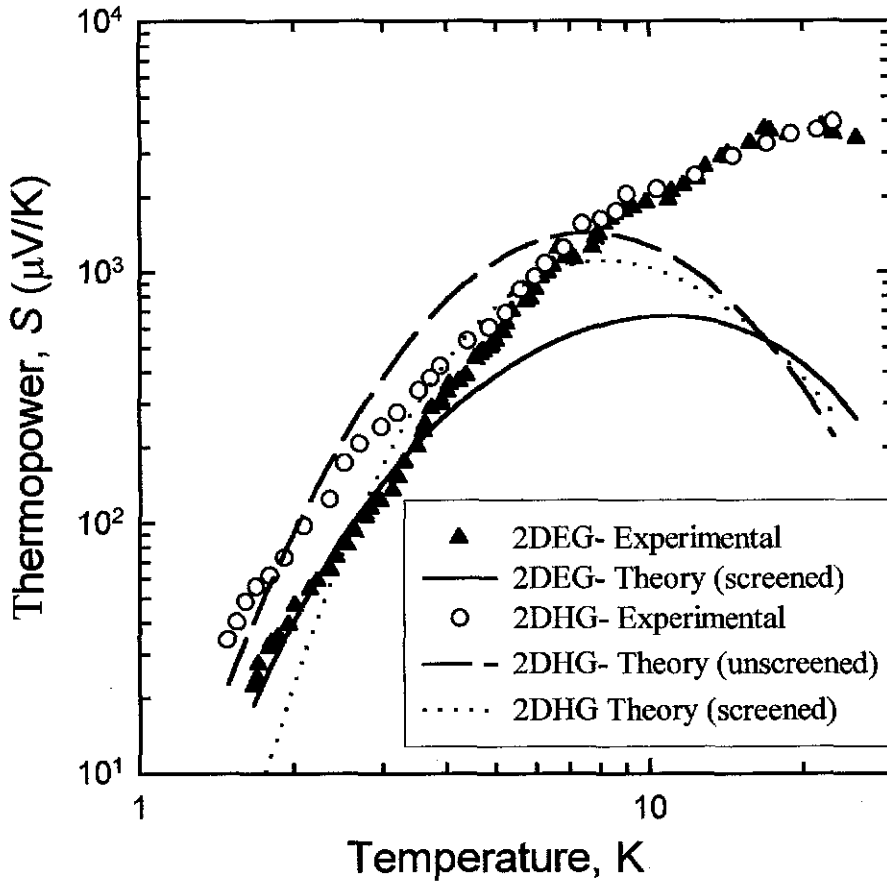


Figure 4.25: Thermopower as a function of temperature for the highest mobility of $2.6 \times 10^5 \text{ cm}^2/\text{V.s}$ 2DEG (Si) sample has $4.5 \times 10^{11} \text{ cm}^{-2}$ sheet carrier density. Deformation potential has been used $\Xi_u = 9 \text{ eV}$ and $\Xi_d = -6 \text{ eV}$ ($g_v=2$) (screened deformation potential). Inverted sample 55.51 (2DHG) Si/Si_{0.8}Ge_{0.2} has $4.7 \times 10^{11} \text{ cm}^{-2}$ sheet carrier density and low mobility of $3.5 \times 10^3 \text{ cm}^2/\text{V.s}$. For 2DHG sample have been fitted using $\Xi=2.5 \text{ eV}$ unscreened deformation potential and 4.5 eV screened deformation potential.

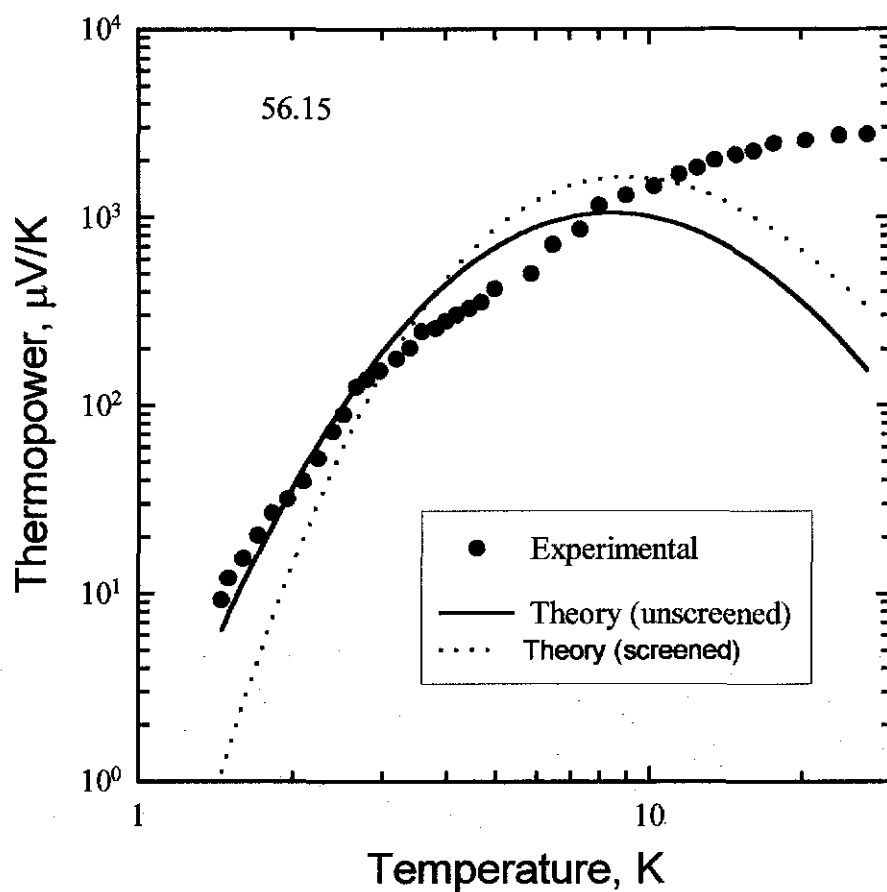


Figure 4.26: Comparison of thermoelectric power as given by the theoretical prediction with experimental data. Normal doped 2DHG Si/Si_{0.8}Ge_{0.2} sample has $7 \times 10^{11} \text{ cm}^{-2}$ sheet carrier density and low mobility of $2.5 \times 10^3 \text{ cm}^2/\text{V.s.}$ The sample has been fitted using $\Xi=2.5 \text{ eV}$ unscreened deformation potential and 4.5 eV screened deformation potential.

4.7 The sheet carrier density dependence of thermopower

One of the most important findings was that if phonon drag is the dominant mechanism for thermoelectric transport then the magnitude of the thermopower should vary inversely to the sheet carrier density of the holes in the 2DHG. **Figure 4.27 (a)** is a plot of 1.5 K thermopower vs. inverse sheet carrier density (as determined from SdH and Hall measurements) for several of our samples. At low values of $1/n_s$, S rises approximately linearly for five 2DHG's over the temperature range in which phonon drag thermopower is expected to dominate. **Figure 4.27 (b)** shows that the thermopower depends on the Fermi Energy of the samples. The corresponding sheet carrier densities are $n_s = (0.8-10.5) \times 10^{11} \text{ cm}^{-2}$. Although the samples exhibit a wide range of mobilities, no correlation with mobility exists. The results reveal some very important features of the 2DHGs under consideration.

4.8 Kohn anomaly of thermopower in Si/SiGe

The "Kohn anomaly" maxima are clearly visible and there is a tendency for higher temperatures as the carrier density is increased. The peaks occur when the dominant phonon wavevector, q_D , coincides with the Fermi wavevector, k_F . In Chapter 2.9 a brief discussion was given about the changes in the strength of the hole-phonon interaction which depend on the phonon wavevector satisfying certain conditions (e.g. $q\ell \geq 1$ and $q\ell \leq 1$). These changes can show up in S/λ_L as a function of temperature wavevector. $q\ell$ is always greater than 1 over the

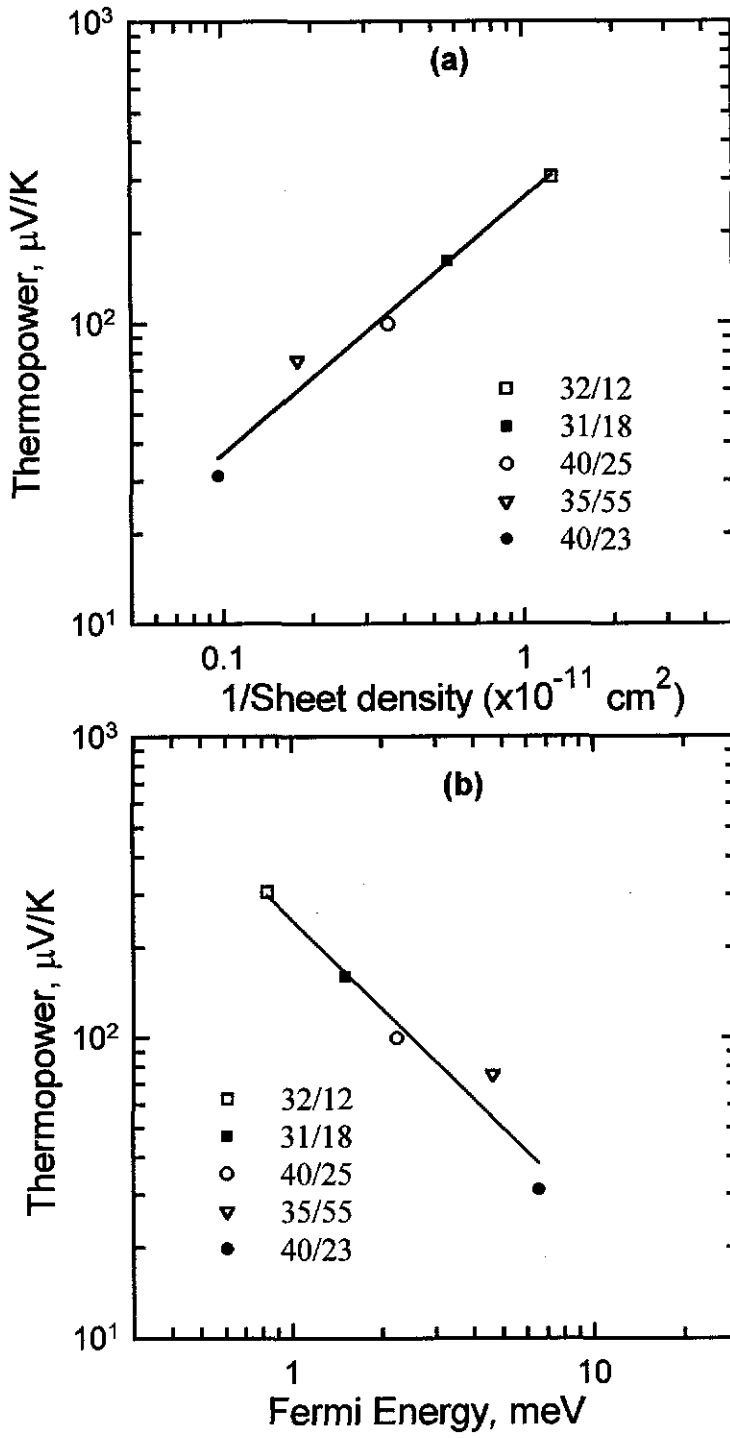


Figure 4.27: (a) The thermopower vs. sheet carrier density for several of our samples. At low values of $1/n_s$ S rises approximately linearly for 2DHGs at 1.5 K. (b) shows low thermopower depends on Fermi Energy of the samples. The lines have gradient 1.

temperature range used, which means that the cut off of most relevance is the one which occurs when q is near $2k_F$. The condition $q=2k_F$ causes a peak in S/λ_L versus T for Si/Si_{1-x}Ge_x heterostructures, due to the enhancement of the hole-phonon interaction.

Figure 4.28 depicts the ratio S/λ_L for sample 31.17. At higher temperatures it shows a maxima in S/λ_L . This indicates the occurrence of a Kohn resonance when the dominant phonon wave vector $q=5k_B T^*/\hbar v_s$ becomes equal to $2k_F$. The temperature at which we expect the maximum is $T_t^* = 2.0$ K and $T_l^* = 2.9$ K which is in agreement with the experimental data. **Figure 4.29** shows theoretical and experimental values of Kohn temperatures (T^{KA} according to v_t (transverse), v_l (longitudinal) and v_s (with arrows) average sound velocities (valley degeneracy $g_v=1$)) for different variation of the sheet density of normal and inverted modulation doped 2DHGs samples. Again, the temperature of the peak increases with n_s , but not as fast as $n_s^{1/2}$. **Figure 4.30** shows S/λ_L depend on effective mass and sheet carrier density (a) and germanium composition (b) at 1.5 K (Zavaritsky, 1984).

4.9 Parallel conduction effects in Si/SiGe heterostructures

The influence of parallel conducting paths on the measured properties of the two dimensional channel should be important in thermoelectric experimentation. If one considers a system composed of parallel layers so that these layers experience a common thermal gradient, simple calculations give the total thermopower as Eq. (2-23) (Zvyagin, 1992). In practice, the parallel layers

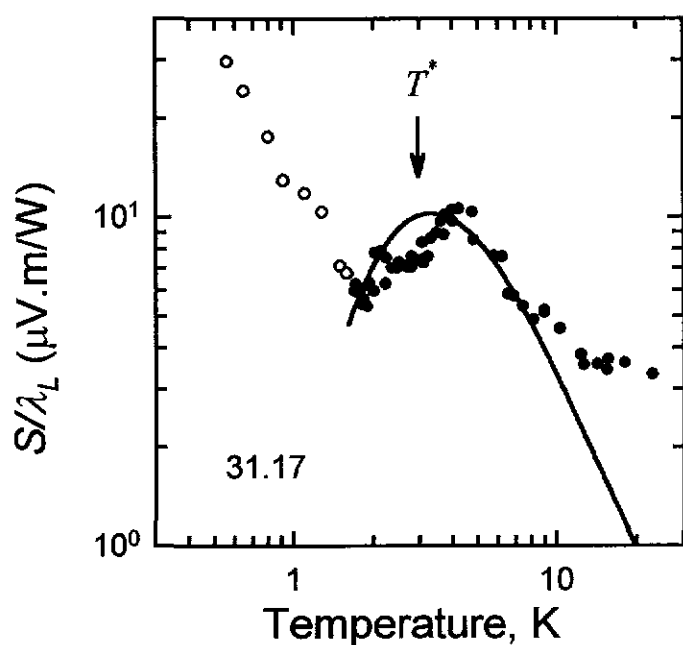


Figure 4.28: The ratio of the thermopower S over the thermal conductivity λ_L as a function of temperature. The circles are the experimental data and solid curve is the theoretical estimation of S_g , divided by the experimental values of λ_L in the temperature range 1.5 – 25 K. The temperature T^* shows the maximum at 3 K.

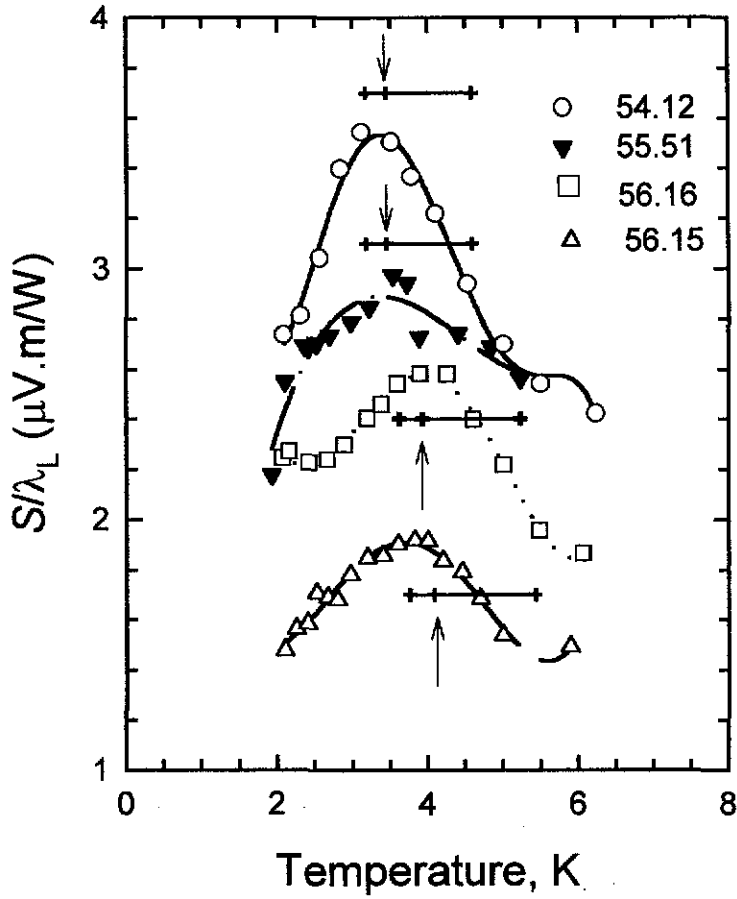


Figure 4.29: The ratio of the thermopower S to thermal conductivity λ_L as a function of temperature for normal and inverted doped 2DHG samples with the parameters given in the Table 4.1-3. The crosses give estimated Kohn temperatures T^{KA} for v_t , v_l and v_s (arrows) taking valley degeneracy $g_v=1$. Here v_t , v_l and v_s are transverse, longitudinal and average sound velocities, respectively. Kohn anomaly temperature T^{KA} , where expected sheet density dependence is clearly observed in the experimental data is shown.

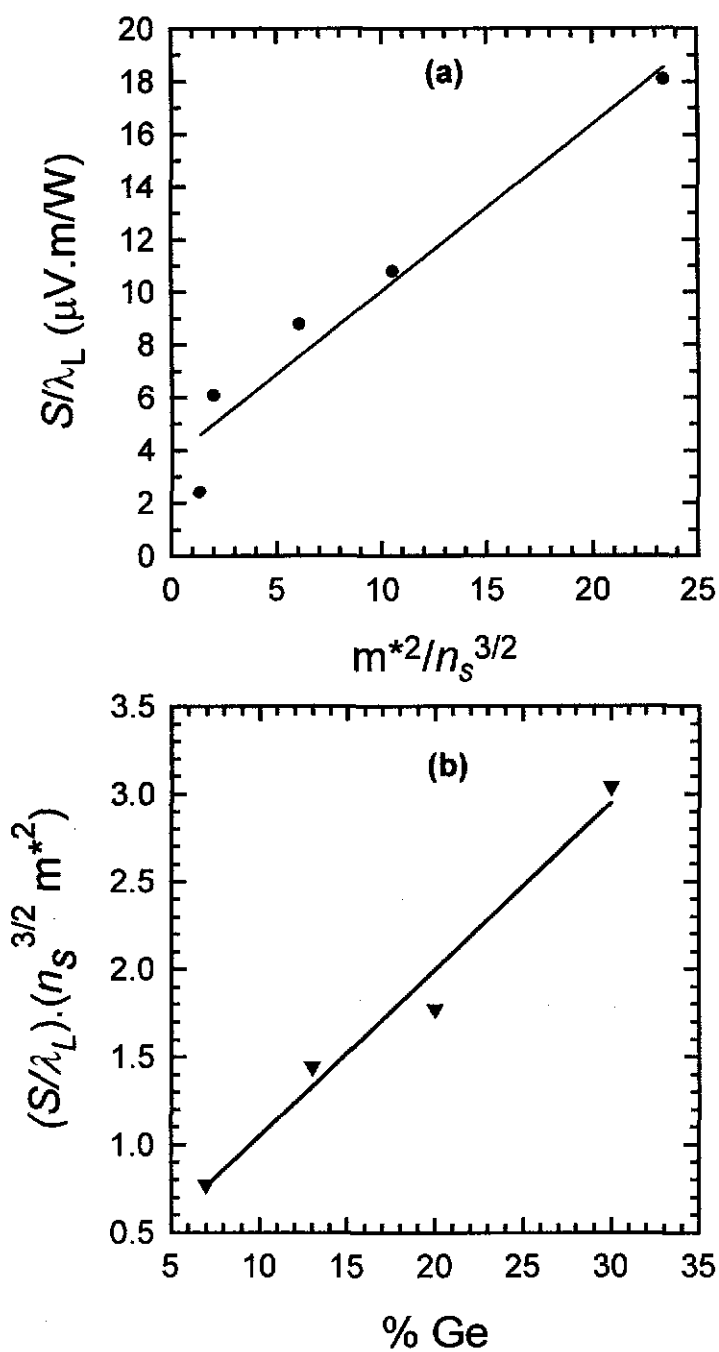


Figure 4.30: (a) S/λ_L depend on effective mass and sheet carrier density and (b) as a function of germanium composition at 1.5 K.

may be different groups of carriers, e.g. electrons and holes, or different subbands, or the combination of the 2DHG or 2DEG and bulk semiconductors.

The experiments have provided a convincing demonstration of the effect of parallel conduction in the doping spike on the 2DHG thermopower. The simple method of investigating the effect of the substrate on the thermopower was simply to compare the measurements of the epilayer away from sample 47.07 and 50.36 in the above studies. The methodology and results of studying the two effects of current concern are discussed separately. Thermopower studies have provided new information on both the hole-phonon interaction for Si/SiGe based 2DHG's and the mobility limiting scattering mechanisms for such devices at room temperature.

4.9.1 Effect of the B doping cap in Si/SiGe

In order to study the contribution of the cap to parallel conduction it was necessary to characterise methodically the thermopower and resistance following the changes which should alter the level of contribution from the cap. Two samples were measured in which the 'cap only' was studied. These were the simple doped epilayer samples in which the epilayer was grown in order to represent as closely as possible the hole donor. **Figure 4.4** shows the resistivity results for epilayer sample 50.36 which is a 50 nm, $2 \times 10^{18} \text{ cm}^{-3}$ boron doped epilayer sample. **Figure 4.31** shows the thermopower results for the same sample. Similarly, the results for 47.07, an epilayer of 50 nm and $3 \times 10^{18} \text{ cm}^{-3}$

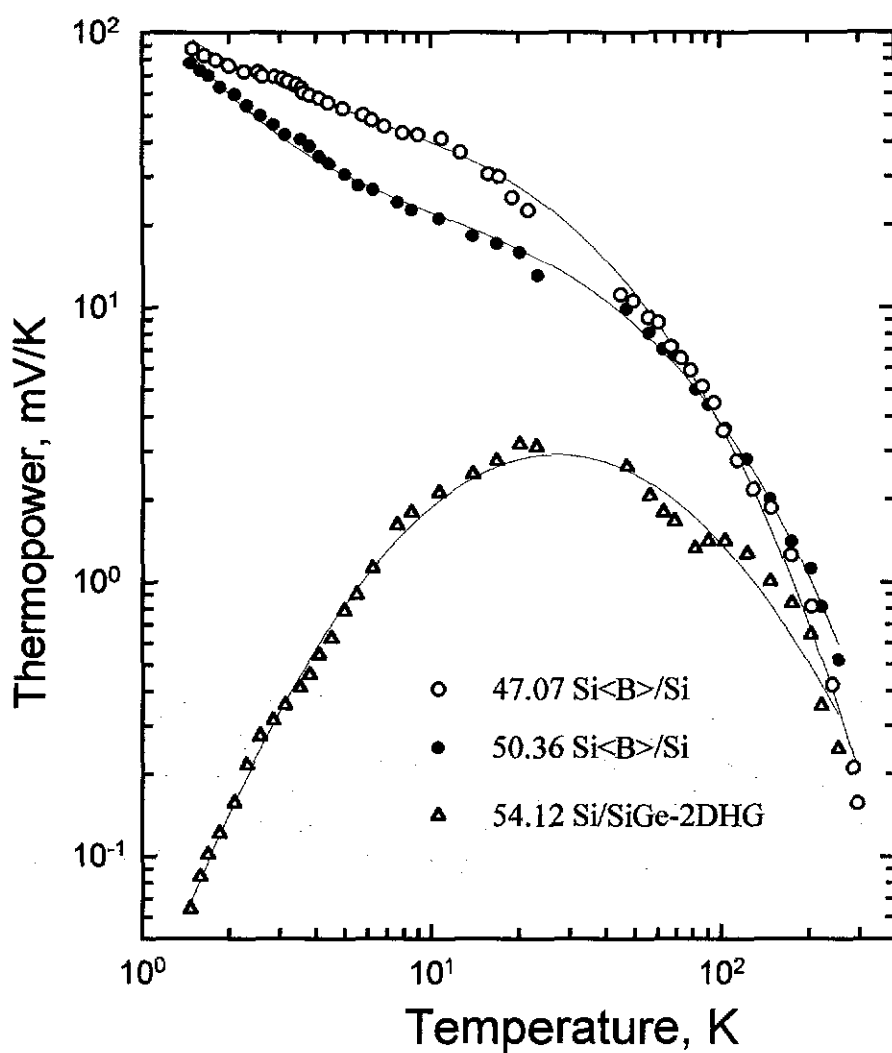


Figure 4.31: Thermopower as a function of temperature for two B doped epilayer (Si:B $2 \times 10^{18} \text{ cm}^{-3}$ (50.36) and $3 \times 10^{18} \text{ cm}^{-3}$ (47.07)) and one Si/SiGe 2DHG (Si:B $2 \times 10^{18} \text{ cm}^{-3}$ 54.12) samples.

boron is also shown in **Figure 4.31**. Clearly, the more heavily doped 47.07 provides the lower resistance path at the lower temperatures where the substrate has frozen out. The magnitude of carrier freezeout is greater, shown by the fact that the channel resistance became greater than $20\text{ M}\Omega$ and in practice was no longer measurable with the available equipment. Further discussion of substrate and contact characteristics will be found below.

The thermopower results for these two samples comply with what might be expected for two samples with varying epilayer resistivity. This is to say that the thermopower of 50.36 is greater than that of 47.07 which is commensurate for a sample of greater resistivity and lower carrier concentration. Hence the inverse relationship of thermopower on carrier density applies. Note also that the magnitudes of the thermopower for these two samples are far greater than generally seen in the 2DHG samples studied.

In the case of a 2DHG, which contains at least the 2D channel and the doping cap, then when at low temperatures the cap freezes out, and the thermopower of the remaining 2DHG will dominate. This has been seen to be the case and is exemplified by comparison of the 50.36 with the 54.12, which contain comparable doping layers (50 nm , $2\times 10^{18}\text{ cm}^{-3}$ and 50 nm , $3\times 10^{18}\text{ cm}^{-3}$ respectively). The results are shown in **Figure 4.31**. The graph for resistance simply illustrates what is commonly known, that the overall sample resistance increases on initial cooling due to the freezing out of the doping layer, and that both the samples follow the same initial trend. At around 100 K though, the

epilayer continues to freeze out, whereas for the 2DHG sample, the holes trapped in the channel suffer fewer mobility limiting impurity collisions.

In **Figure 4.31**, the thermopower results are similar at high temperatures. However, at low temperatures where the doping spike has effectively frozen out in 54.12, the thermopower is dominated by the thermal voltage of the lower resistance 2DHG and is around three orders of magnitude smaller than that for the doping layers on their own of samples 50.36 and 47.07. As a result, such a contribution would decrease with decreasing temperature. In **Figure 4.32**, full circles represent thermopower results of the epilayer sample 50.36 and open the triangles results represent those of the 2DHG sample 54.12. Both samples have $2 \times 10^{18} \text{ cm}^{-3}$ B doping. The solid line is calculated according to the formula (2-23). It is clear that there is no significant parallel conductance below 10 K and starting slightly above 10 K.

4.9.2 The effect of the Si substrate in Si/SiGe

The simple method of investigating the effect of the substrate on the thermopower was to compare the measurements before and after entirely etching away the epilayer from the sample 50.36 studied above. By contacting through the epilayer and then etching the epilayer away (protecting the contacts), the structure of **Figure 4.33** was left. A comparison is possible between identical structures (i.e. the same sample) with the epilayer present and without. The removal of the epilayer isolates the contribution to the resistivity and thermopower of the substrate. The second objective achieved is of greater

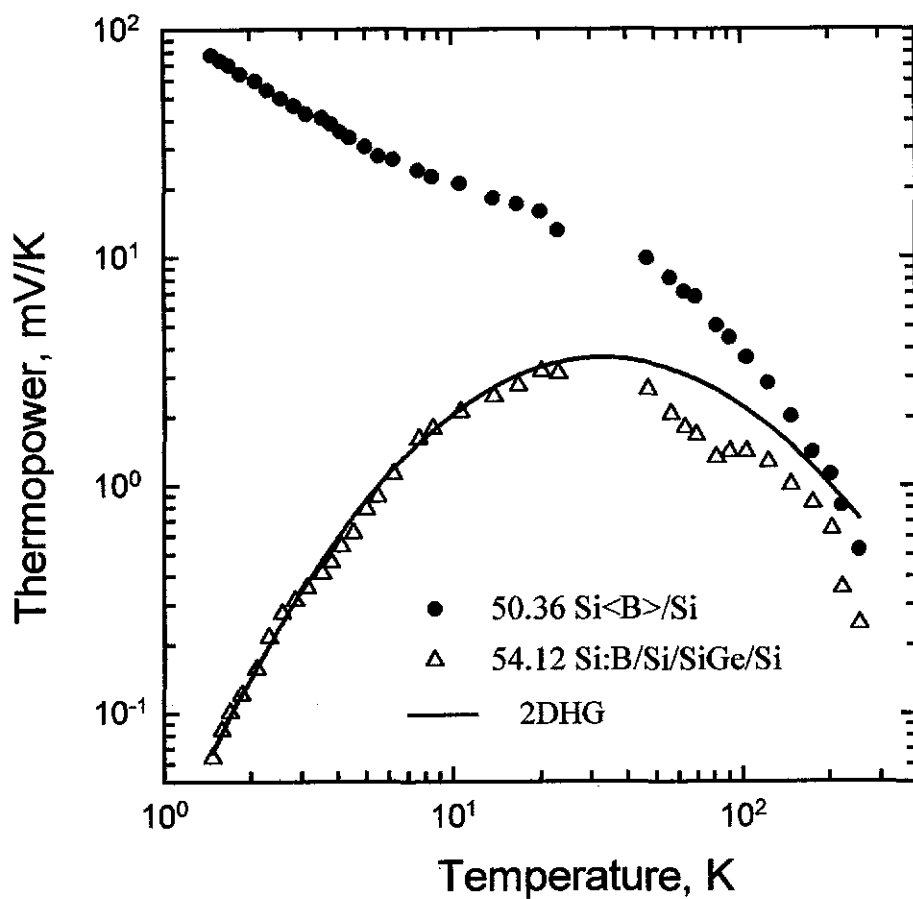


Figure 4.32: Thermoelectric power S vs. temperature T . The circles are the experimental data of epilayer sample (Si:B/Si). The triangles are Si:B/Si/Si_{0.8}Ge_{0.2}/Si. Solid line is 2DHG extracted from Eq. (2-23). It is clearly seen that there is no any contribution to the thermopower from B doped layer at He⁴ temperatures.

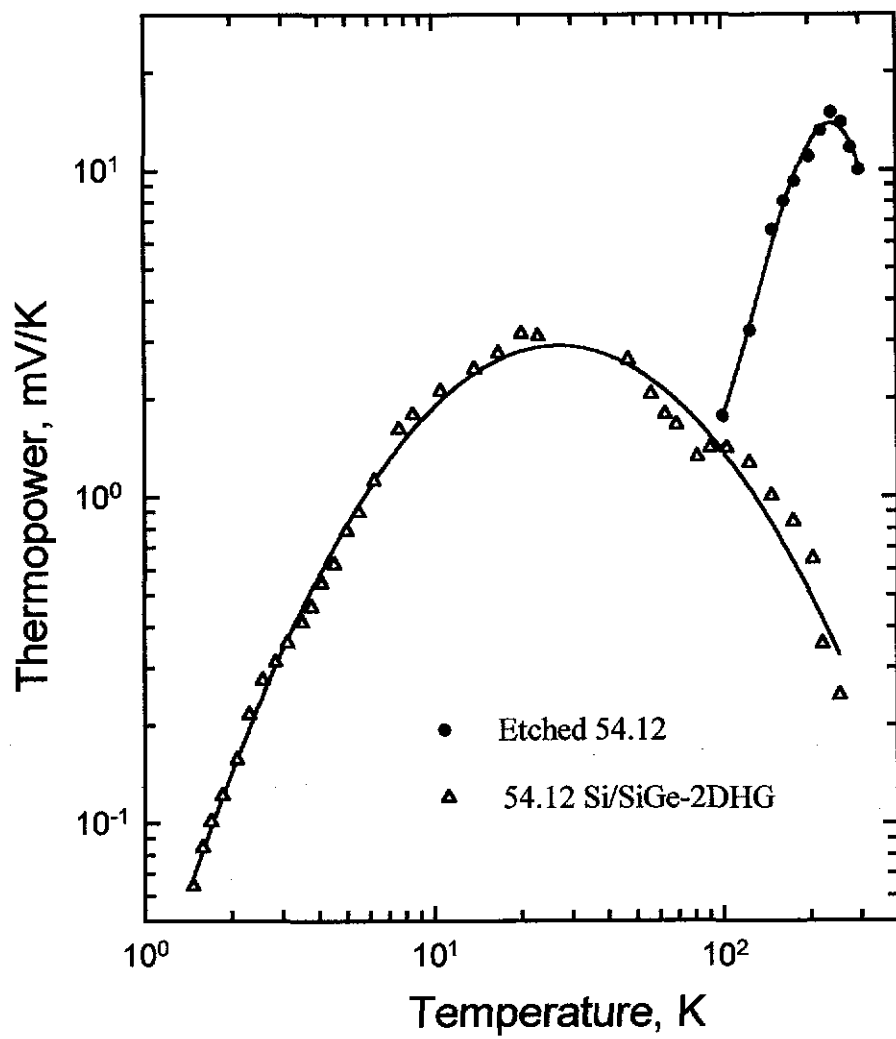


Figure 4.33: Thermopower as a function of temperature with and without etched Si:B doping layer for Si/SiGe 2DHG (Si:B $2 \times 10^{18} \text{ cm}^{-3}$ 54.12).

significance the contact structure is not ideal for measurements on the substrate since the contact is p-type and the substrate n^- .

Following etching, the contacts were rectified. This would clearly be hoped for (p-type contact to n^- type substrate) and by 100 K the resistance of the sample could no longer be measured. As a result of, the substrate was supposed to have no effect on the measurements of either resistivity or thermopower since adequate electrical contact was absent. The fact that the heterojunctions have conducting bulk layers may lead to a contribution to the thermopower in two ways, but neither of these is expected to influence greatly below 30 K which is the case for all the 2DHG samples measured.

4.10 Discussions and conclusions

The electrical properties for normal and inverted modulation doped Si/SiGe/Si structures of the 2DHG are set out in this chapter. The holes were supplied to the strained SiGe quantum channel well by a boron doped layer spatially separated from the alloy.

The diffusion thermopower in the metallic regime is relatively well understood. This gives essential information on electron scattering, as well as a unique contribution which arises from the dependence of S on the energy derivative of the scattering time τ . The behaviour of our 2DHG was in accordance with phonon-drag Cantrell-Butcher theory in the temperature range 1-10 K. The diffusion thermopower was dominant below 1.5 K. We have seen the diffusion thermopower ($S \sim T$) below 1.5 K for sample 31.17. Theoretical

calculations of Mott diffusion term show that it is negligible over the entire degenerate range of measurements above 1.5 K. We therefore discuss the possibility that the discrepancy between the measurements and the deformation potential theory can be accounted for by a piezoelectric scattering contribution to the phonon drag thermopower (Xie *et al.*, 1986).

Experimental and theoretical investigations of the thermoelectric power for 2DHG's in Si/SiGe heterostructures and 2DEG revealed a number of important features. There is new evidence to suggest the existence of some type of alloy ordering such that piezoelectric scattering of holes may be significant in certain samples. A systematic study is necessary to reveal which material parameters are responsible for this effect. Values for the effective acoustic deformation potential in SiGe alloys of different compositions have been found which agree with both previous experimental and theoretical consideration of mobility limiting scattering in SiGe channels. The value of the parameter p in the theory of diffusion thermopower has been established and suggests that the mobility in at least some of our samples is limited by remote ionised impurity scattering at high temperatures.

Certainly, there is good evidence for the presence of phonon drag based on the results of the sheet density variation study. Evidence for the dominance of the substrate doping on the thermal conductivity is also given (see **Figure 4.18**).

CHAPTER FIVE

RESULTS FOR AND <Sb> DELTA LAYERS IN SILICON

5.1 Introduction

In recent years, the doping of semiconductor structures down to atomic resolution (atomic layer doping (ALD) or δ -doping) has become possible (Schubert, 1996). Delta-doped structures are suitable systems for the study of physics at extremely high carrier densities, and for potential device applications such as δ -FET (Schubert, Fischer and Ploog, 1986, and Nakagawa, van Gorkum and Shiraki, 1989). This study is concerned with the properties of the so called “ δ ” (delta) doped system which represents the ultimate scaling down of the dimensions in one direction to one atomic plane.

The delta layers can be used with a number of novel devices incorporating two dimensional electron or hole gases (Biswas *et al.*, (1993); Matthey *et al.*, (1992a, b); Whall, (1992); Gossman and Schubert, (1993) and delta MOSFETs (Schubert, 1990b). The study of the thermopower informs us of various

scattering mechanisms of importance over the full range of temperatures from 1.5 K to room temperature.

In this study, measured samples were characterised by the XRD, SIMS and Hall effect. Matthey *et al.*, (1992b) shows B δ -layer which is ~ 2 nm. To provide further information on the δ layer width cross-sectional, TEM was used. Preliminary analysis was performed on a B δ -layer of areal density $1 \times 10^{13} \text{ cm}^{-2}$ (Matthey *et al.*, 1990a).

Thermoelectric power measurements provide valuable data which determine parameters for device modelling, such as the value of deformation potential. In this work, we have measured thermopower (S) and thermal conductivity (λ_L) on a series of delta-boron (p -type) and delta-antimony (n -type) doped (001) Si structures with hole P_s and electron n_s sheet densities in the range $(0.3\text{-}1.05) \times 10^{14} \text{ cm}^{-2}$.

5.2 Hall effect results for delta B doped samples

Boron delta layers were deposited on a Si wafer in a modified VG Semillon V90S MBE system fitted with an elemental boron evaporation source in which the residual gas pressure during growth was 10^{-9} mbar. The substrates were low doped n^+ silicon of 100 mm diameter. After the substrates were prepared at 850 °C, 300 nm of undoped Si was deposited at which point the temperature was reduced to 480 °C. The substrate was then exposed to a boron flux of $6 \times 10^{11} \text{ atoms cm}^{-2} \text{ s}^{-1}$ for a certain predetermined length of time whilst

the Si source was shuttered; the resulting doping spike was then buried beneath a capping layer of 75 nm of undoped Si.

Van der Pauw method has been used for the electrical measurements. The variation of sheet resistivity $R_{\square}$ with temperature T is shown in **Figure 5.1**. The various curves are for samples with different B doping concentrations p_s in the δ -layer. The variation of carrier density p_s with temperature is shown in **Figure 5.2**. From 300 K down to 100 K the carrier concentration, as obtained from the Hall effect, gradually decreases with temperature. As the doping concentration p_s in the δ -layer increases, this variation becomes relatively flat and at $p_s \approx 1 \times 10^{14} \text{ cm}^{-2}$ it is independent of temperature. Samples with $p_s \approx 10^{13} \text{ cm}^{-2}$ show a rise in p_s at temperatures between 100 and 50 K. Below 50 K, p_s is almost independent of temperature.

The electrical properties of the B delta-layers were studied by means of the temperature dependent Hall effect and resistivity measurements were carried out between 1.6 and 300 K. **Figure 5.3** shows the variation of Hall mobility μ_H with temperature. As the temperature goes down from 300 K to about 120 K μ_H , assuming a single type of carrier, the temperature slowly increases for all the samples. It then rapidly decreases with the further fall of temperature and finally becomes constant at $\leq 50 \text{ K}$. Interpretation of the Hall measurements is complicated by the multi-subband conduction, although Eisele (1989) has argued that the measurement leads to a minimum value.

Syme and Kearney (1992) have thoroughly examined the nature of weak localisation and electron-electron scattering in a highly disordered system and

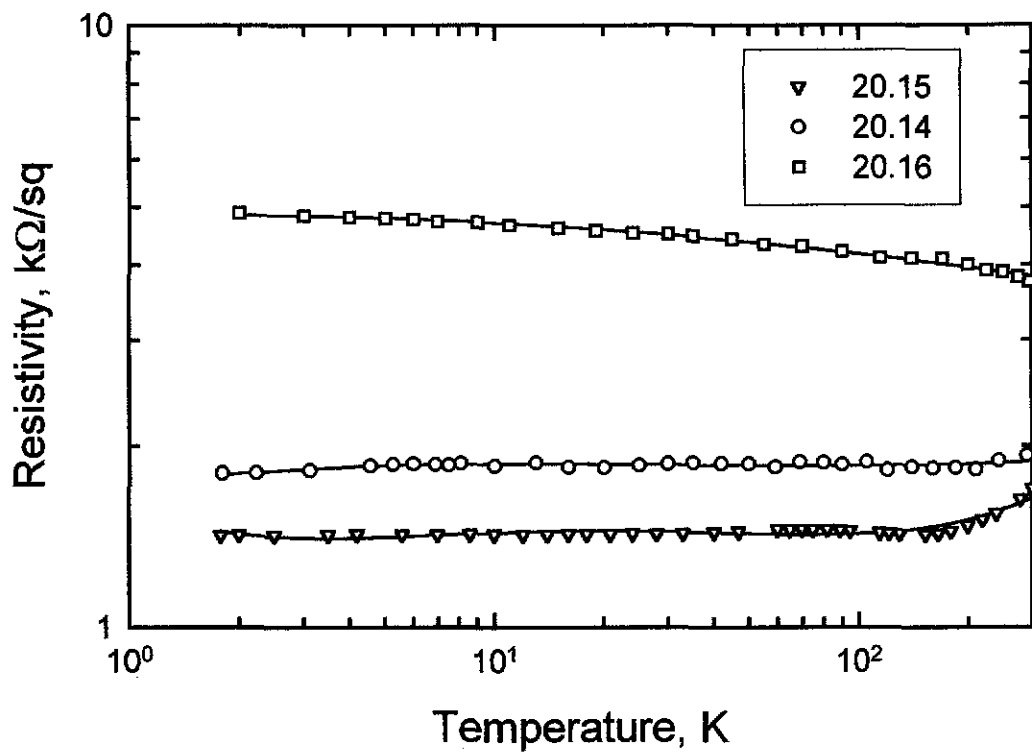


Figure 5.1: Variations of sheet resistivity with temperature of delta B doped samples.

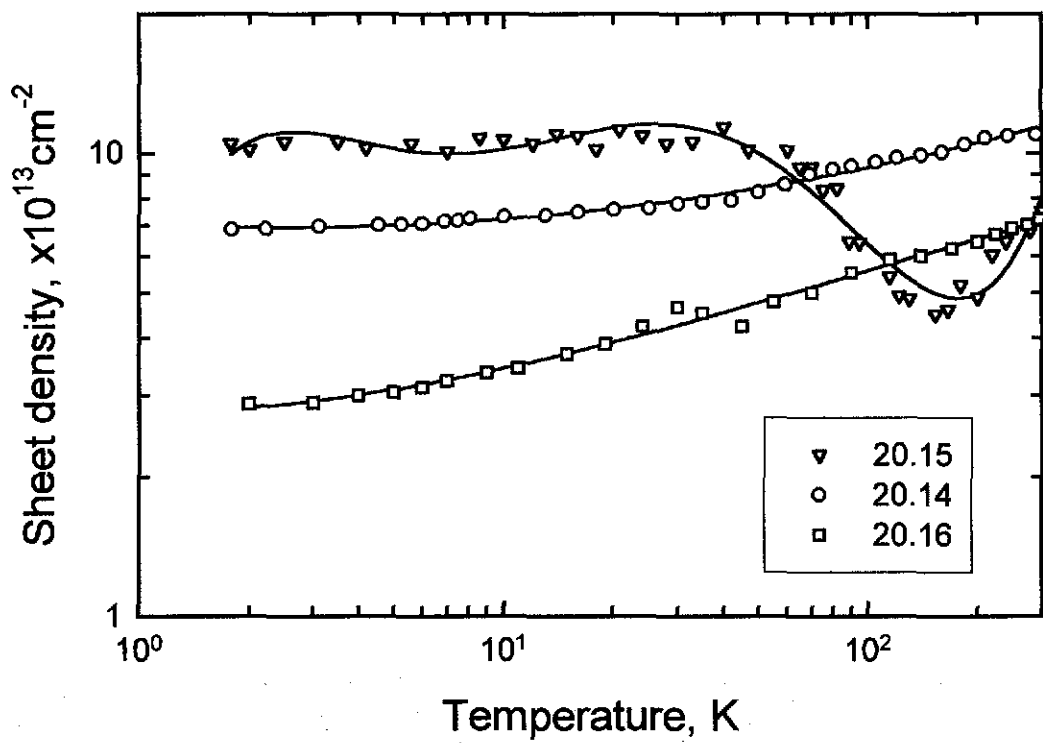


Figure 5.2: Variations of carrier density p_s with temperature.

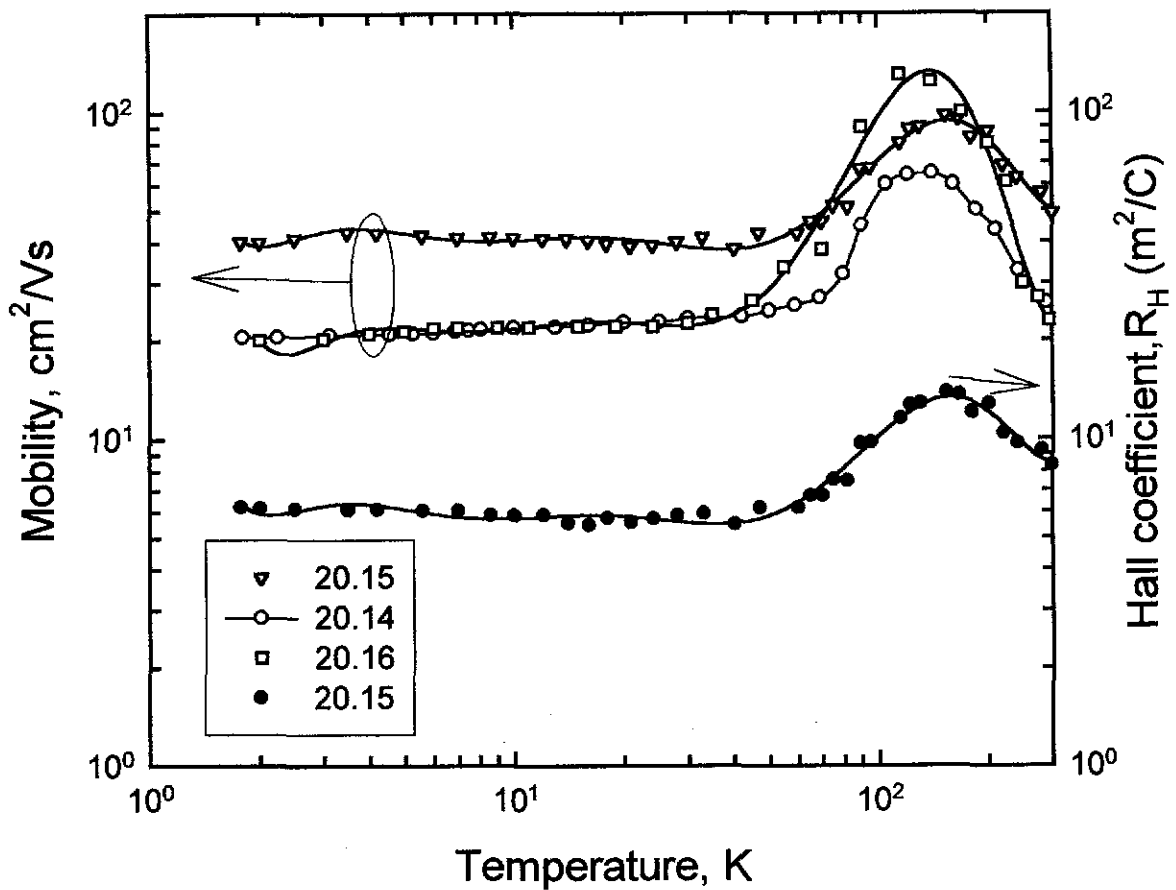


Figure 5.3: Hall mobility vs. temperature of delta B doped samples and Hall coefficient, R_H of sample 20.15 with $1 \times 10^{14} \text{ cm}^{-2}$ carrier density at 4.2 K. The solid lines guide for eyes.

concluded that the effects of weak localisation and electron-electron scattering were masked by the phonon drag and may only be revealed on the magnetothermopower.

5.2.1 Scattering processes of δ doped Si

For the uniformly doped Si sample with a very low doping, Hall mobility of the carriers is normally limited by the lattice phonon scattering in the high temperature region above room temperature (≥ 300 K) (Pearson and Bardeen, 1949), and by the ionised impurity scattering in the low temperature region (≤ 300 K). In the former case, μ_H should show a $T^{-3/2}$ dependence and in the latter case, a $T^{3/2}$ dependence.

In the case of delta-doped samples, an important difference exists. Here, a large number of impurity atoms are concentrated over a fraction of a monolayer of atoms and thus the ionised flaws are numerous in a localised region of the epilayer. In the presence of both the lattice phonon and ionised impurity scattering, the latter should dominate and lead to a temperature dependence of $\mu_H \propto T^x$ with $x \sim -0.5$ (Blakemore, 1985). This has actually been observed in our samples with higher doping levels in the temperature range 150-300 K where x is found to lie between -0.4 and -0.5 . This agrees with the theory. In the low temperature region between 50-100 K, the influence of lattice phonon scattering should diminish and mostly ionised impurity scattering in addition to other similar mechanisms may take-over leading to $x \sim 3/2$. In our samples, we found x to lie between 1.2 and 2.6 in this temperature region (Figure 5.3).

5.3 Low temperature electron transport in Si- δ <Sb> layer

The studies of the electrical properties of Si single crystals with δ <Sb>-layers of various sheet densities, n_s , of Sb atoms ($5 \times 10^{12} - 9.5 \times 10^{13} \text{ cm}^{-2}$) have provided details of the low temperature features of the electron transport. The number of size-quantized subbands and their filling are determined by the sheet density of impurity atoms. Usually only a few subbands are filled, and the mobility of charge carriers are strongly dependent on the number of the subband. The nature of the subband filling and the mobility of charge carriers were the object of initial studies of δ -layers (mainly of δ <Si>-layers in GaAs) (Zrener *et al.*, 1986; Koenraad *et al.*, 1993 and Panaev *et al.*, 1993).

The transport mobility of the electrons is lower in δ -layers than in modulation doped heterojunctions because impurity scattering is determined by the same impurity atoms which formed the δ -layer. However, δ -layers are distinguished by an important and valuable feature: they allow an arbitrary density of two-dimensional electrons at very low sheet density values ($\approx 10^9 - 10^{10} \text{ cm}^{-2}$), for which the conductivity in the δ -layer ranges from an “hopping” type, to very high values ($\approx 10^{14} \text{ cm}^{-2}$) in which metallic conductivity is realized. This feature of δ -layers provides a unique opportunity to study the effect of the concentration of two-dimensional electrons on the relaxation and interaction of electrons in a two dimensional electron gas and on the character of the transition from metallic to hopping conductivity. For δ <Sb>-layers in silicon, this transition occurs in the range from 0.01 monolayer (ML) of Sb atoms to 0.05

ML in the δ -layer, which corresponds to the electron densities of 6.7×10^{12} to $3.35 \times 10^{13} \text{ cm}^{-2}$ (van Gorkum, Nakagawa and Shiraki, 1989).

5.3.1 Sample details and measuring techniques

The Sb δ -layers were prepared by low temperature silicon molecular beam epitaxy on Si (100) substrates. A 300 nm Si buffer layer was first grown with a substrate temperature of 750 °C and then the Si source was shuttered and the antimony source unshuttered allowing antimony to accumulate on the wafer surface. The antimony deposition is followed by a Si capping layer at a substrate temperature of 250 °C, (and below, avoids Sb profile smearing by surface segregation) (Jorke *et al.*, 1989; Powell *et al.*, 1991). The structure was then annealed at 800 °C in order to activate the antimony delta layer.

The configuration of the impurity region meets the requirements of galvanomagnetic measurements (a narrow strip with current and potential leads forming contact areas on the crystal surface). The results of measurements on the five samples investigated: the pre-assigned concentration n_s of impurity Sb atoms, the resistance $R_{\square}$, and the Hall concentration n of mobile charge carriers at 18 K are given in the Table I. According to precision X-ray diffractometry, the «structural» thickness of the δ -Sb-layers at $n_s = 2 \times 10^{14} \text{ cm}^{-2}$ is below 2 nm (Powel *et al.*, 1990a). A similar result was obtained from secondary ion mass spectrometry and transmission electron microscopy (Zeindl *et al.*, 1987).

5.3.2. General picture of changes in kinetic characteristics

Figure 5.4. shows that the temperature dependences of resistance, $R(T)$, for the samples studied. In the low temperature region, samples 20.22, 20.21 and 20.23 display a very weak increase in resistance as the temperature decreases (Figure 5.4.a). We show that the change is due to the interference effects of weak localization (WL) of electrons and the electron-electron interaction (EEI).

As the temperature rises, the dependencies $R(T)$ change for all samples: the resistance decreases sharply with increasing temperature (Figure 5.4.b). In the samples with lower resistance, the transition temperature T^* rises (e.g., for sample 20.25 the typical value of T^* is ~ 16 K; for samples 20.24, 20.21, 20.23 and 20.22, it is about 25, 35, 50, 60 K, respectively). Variations of the resistance above these temperatures are described well by the relation

$$R = R_1 \cdot \exp (E_1/k_B T). \quad (5-1)$$

The dependence on temperature suggests that in this region conductivity is controlled by the activation of impurity carriers. The estimated values of activation energy E_1 are given in Table 5.1. As the temperature goes above the region described by Eq. (5-1), the dependence $R(T)$ changes: the resistance has a minimum and then grows weakly (Figure 5.4.b). The growth is due to scattering of the activated electrons by acoustic phonons under the condition of the depletion of donor centres.

Thus, at high temperatures there is a competition between the conduction of the δ -layer and the electrons in the conduction band, which are in thermal equilibrium with the electrons at the donor centers. The conductivity of the δ -

layer itself is determined by the overlapping wave function tails of the electrons localized at impurities. **Table 5.1** contains the values of $n_s^{-1/2}$ (Å) characterizing the mean distance between the ionized Sb atoms in the δ -layer.

It is known that under certain conditions electrons can hop from one impurity atom to another by thermally activated tunnelling, without a transition to the conduction band. Although the mobility of the electrons hopping over the impurity levels is quite small, because it is influenced by the interaction of widely separated impurities, at low temperatures the conduction through impurities becomes dominant due to the “freezing-out” of electrons in the conduction band. The resulting specific electric conductivity is (Shklovskii and Efros, 1984):

$$\rho^{-1}(T) = \rho_1^{-1} \exp(-E_1/k_B T) + \rho_3^{-1} \exp(-E_3/k_B T) \quad (5-2)$$

where the first term describes the band conductivity, and the second term corresponds to the hopping-type conductivity with the activation energy constant E_3 . The latter term has its origin in the scatter of impurity energy levels: the transition of an electron from one impurity atom to another is possible when phonons are absorbed or emitted. It is seen in **Figure 5.4.a** that at lower temperatures the dependence of temperature on resistance as described by Eq. (5-1) with the activation energy E_1 changes for sample 20.24 and 20.25. A temperature region appears in which the second term of Eq. (5-2) with low activation energy E_3 becomes dominant. According to experimental results, it is 3.9 meV. This exponential dependence is evident around ~10 K.

After further decreases in temperature, the temperature dependence deviates from the above exponential behavior due to hopping-type conductivity

with a varying length of the jump (variable range hopping) (Shklovskii and Efros, 1984). At very low temperatures, the hopping conductivity is characterized mainly by states with energies within a narrow band near the Fermi level and the width of this band decreases with lowering temperature. The states within this band are further apart with the length of the jumps increasing as $T^{-1/4}$ and the activation energy decreases as $T^{3/4}$. The temperature dependence of the specific resistance takes the form (Mott's law):

$$\rho(T) = \rho_0 \exp (T_0/T)^{1/4} \quad (5-3)$$

where $T_0 = \beta/k_B v(\mu) a^3$, $v(\mu)$ is the density of states at the Fermi level, and $\beta = 21.2$ (Shklovskii and Efros, 1984; Mott, 1968) is a numerical constant. For a two-dimensional system, Mott's law for variable range hopping is (Brenig, Dohler and Heyszenau, 1973)

$$\rho(T) = \rho'_0 \exp (T'_0/T)^{1/3} \quad (5-4)$$

where $T'_0 = \beta'/k_B g'(\mu) a^2$, $g'(\mu)$ is the two-dimensional density of states at the Fermi level and $\beta' = 13.8$.

The analysis of experimental results for sample 20.24 shows that below 11 K the experimental points fall on a straight line in $\ln R \sim T^{-1/3}$ coordinates (Figure 5.4.c). (Note that in the $\ln R \sim T^{-1/4}$ coordinates the fit to a straight line is not as good.) Thus, in sample 20.24 a decrease in the temperature leads first to the hopping-type conductivity with the constant activation energy and then to the variable-range hopping conductivity.

The analysis of the low temperature conduction of the samples investigated and the dependence of the resistance $R_{\square}$ on the Sb atom density in

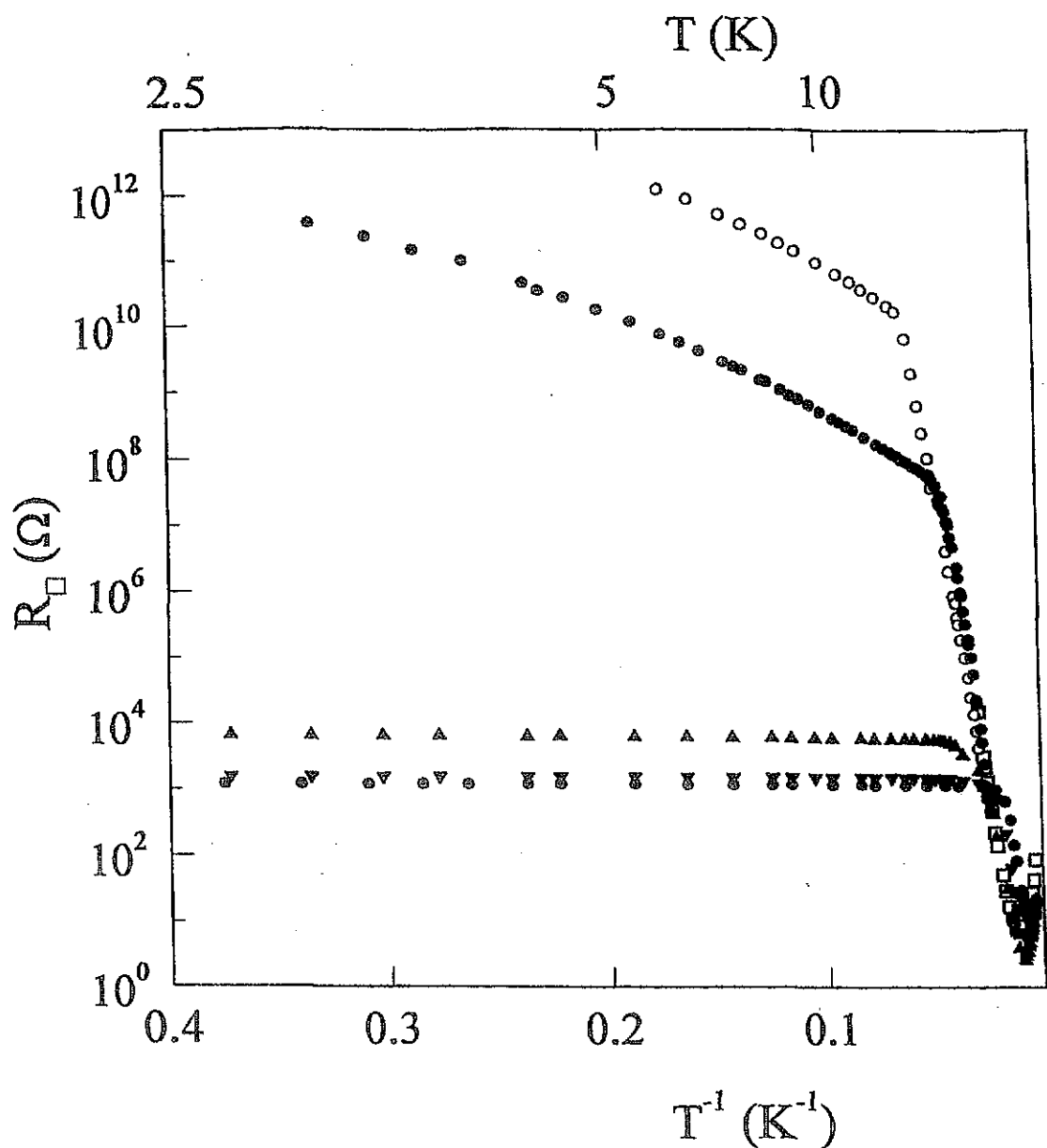


Figure 5.4: $R(T)$ dependencies for samples 20.22 (1), 20.21 (2), 20.23 (3), 20.24 (4) and 20.25 (5). The general picture of resistance variations is shown in the low temperature region in the $\ln R_{\square} - T^{-1}$ coordinates (a), at intermediate temperatures (b) and resistance variation of sample 20.24 in the low temperature region in the $\ln R_{\square} - T^{-1/3}$ coordinates (c).

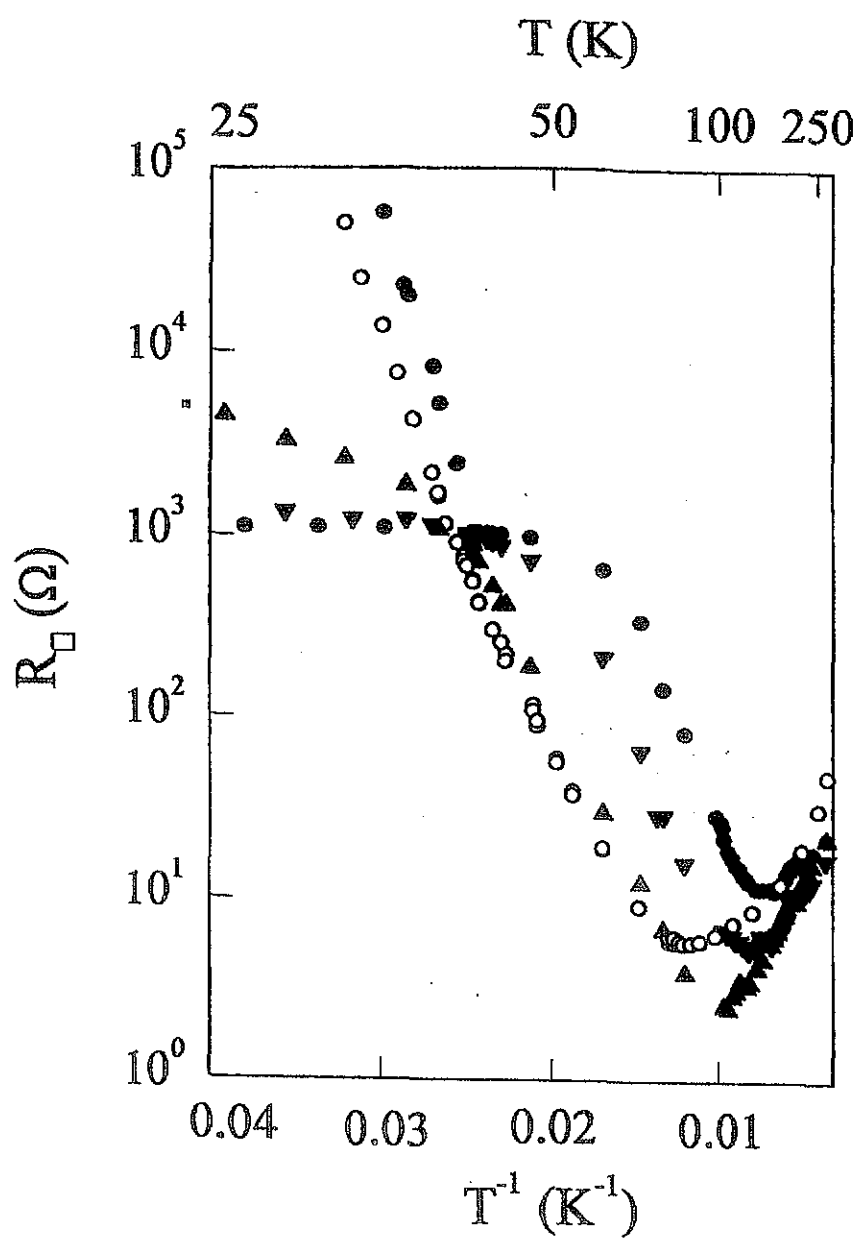


Figure 5.4 (b)

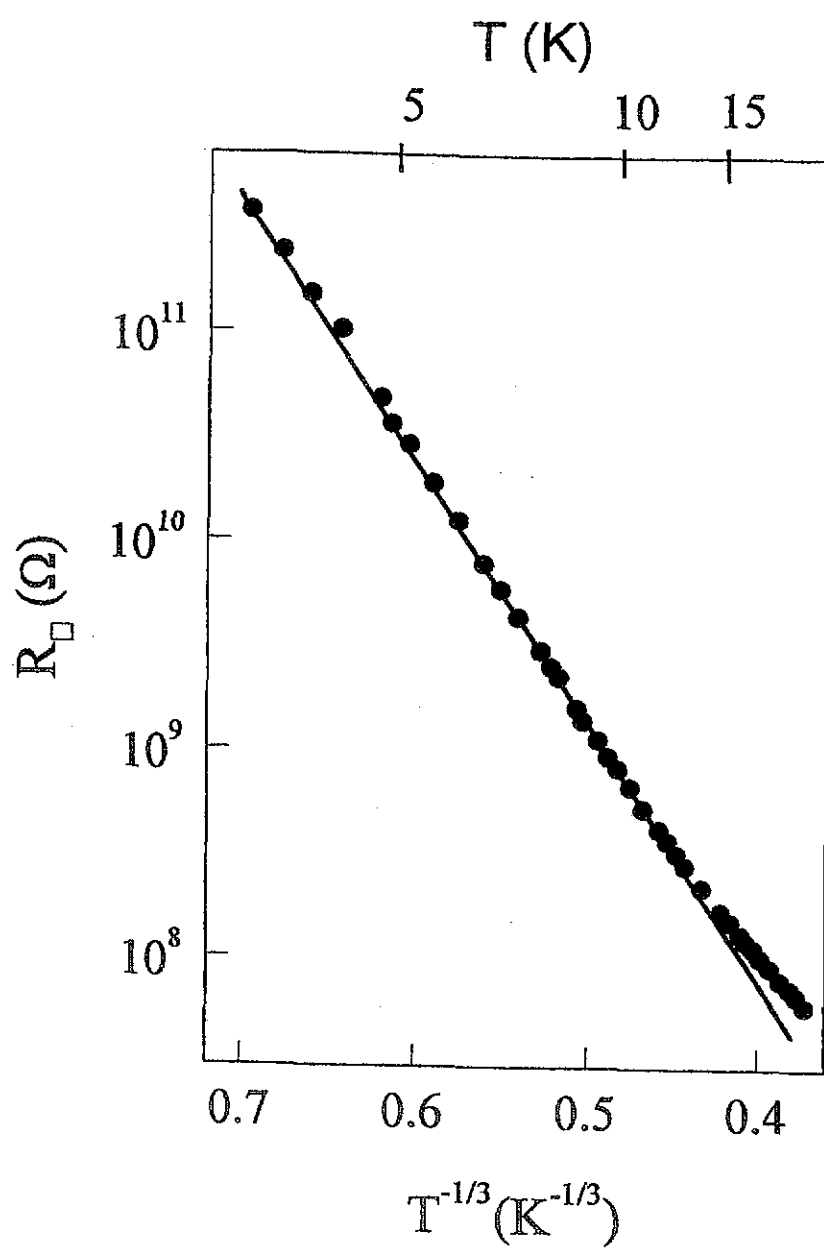


Figure 5.4 (c)

the δ -layer (see the Table 5.1:) shows that the metal-insulator transition (MIT) occurs at $N_D \leq 3 \times 10^{13} \text{ cm}^{-2}$: samples 20.22, 20.21 and 20.23 are on the metallic side, and samples 20.24 and 20.25 are on the insulator side of the transition. This agrees with the results in Ref. (van Gorkum, Nakagawa and Shiraki, 1989) which shows that the MIT takes place in the range 0.01- 0.05 ML of Sb atoms in the δ -layer. The metal-insulator transition was earlier observed on Si samples with δ -layer of boron, which is an acceptor impurity (Mattey *et al.*, 1992b). In that case the MIT occurs at $p_s \sim 1 \times 10^{13} \text{ cm}^{-2}$.

5.3.3 Electron-phonon relaxation

The effect of electron overheating (Shklovskii, 1980) can be used to find the electron-phonon relaxation time, τ_{ep} . As a result of electron overheating by the electric field, the transfer of excess energy from the electrons to the lattice is dependent on the time of the electron-phonon energy relaxation. The advantage of this method is that τ_{ep} can be estimated in the temperature interval where electron-electron scattering is predominant among the inelastic processes of relaxation.

In the δ -layer, the electrons are two-dimensional since they occupy quantum levels in a certain potential well and have momentum vectors lying in plane cross sections in reciprocal space. The phonons that interact with electrons, however, are three-dimensional, and their interaction with electrons involves the component of the phonon wave vector out of the 2D plane. The kinetic characteristics of 2D and 3D electrons differ only in their numerical

factor (Price, 1981) since 2D electrons have a lower possibility of changing their momenta. We may assume that the functional dependencies $\tau_{ep}^{-1}(T)$ at $q_T\ell > 1$ and $q_T\ell < 1$ are similar in character for 2D and 3D systems.

Table 5.1: The parameters for the studied Si delta-Sb doped samples.

Parameter	Samples				
	20.22	20.21	20.23	20.24	20.25
n_s, cm^{-2}	$3 \cdot 10^{14}$	$1 \cdot 10^{14}$	$3 \cdot 10^{13}$	$1 \cdot 10^{13}$	$5 \cdot 10^{12}$
$n_s^{-1/2}, \text{\AA}$	5.7	10	18	32	45
$R_{\square}^{4.2\text{K}}, \Omega$	$1.17 \cdot 10^3$	$1.53 \cdot 10^3$	$4.81 \cdot 10^3$	10^9 (at 8 K)	$2 \cdot 10^{11}$ (at 8 K)
n_s, cm^{-2} (at 18 K)	$9.5 \cdot 10^{13}$	$7.8 \cdot 10^{13}$	$3.1 \cdot 10^{13}$	$1.5 \cdot 10^9$	-
E_1, meV	42	41	37	44	44
λ_T^D	0.93	0.90	0.60	--	--

5.4 Lattice thermal conductivity measurements

The thermal conductivity of silicon is dominated by phonon transport and can be reduced by phonon scattering on the boundaries. For these measurements, an electrical current of 0.5 - 7 mA was applied to the top heater during the He^4 temperature measurements (1.5 - 25 K). For liquid N_2 temperatures up to room temperature, a current of 25 mA was applied to the top heater. ∇T temperature gradients were then obtained for each current. **Figure**

5.5.a shows temperature difference dependence of the top heater current at 1.5 K for the 2DHG sample 20.15. Temperature difference vs. heater power is illustrated in **Figure 5.5.b**.

Thermal conductivities versus temperature measured for various doping compositions from **Table 5.2** are displayed (2DHG) in **Figure 5.6**. and three delta antimony doped samples (2DEG) in **Figure 5.7**. The Sb delta doped sample have p^- substrate with $(4.9-7.1) \times 10^{15} \text{ cm}^{-3}$ doping concentration and $(3-9.5) \times 10^{13} \text{ cm}^{-2}$ sheet density while the B delta doped samples have same type n^- substrate with $(1.7-2.7) \times 10^{15} \text{ cm}^{-3}$ doping concentration and $(3-10.5) \times 10^{14} \text{ cm}^{-2}$ sheet density. Effective mass of these samples is approximately $m^*=0.56 m_0$ (Mattey *et al.*, 1992b) and delta layer is $\sim 3 \text{ nm}$ (Mattey *et al.*, 1990b).

Table 5.2: The parameters for the studied Si delta-B and delta-Sb doped samples

Hall effect sheet density n_s, p_s (10^{13} cm^{-2}) @4.2 K $n_s = (e R_H)^{-1}$	FWHM (nm)	Growth temperature (K)	Cap layer thickness (nm)	Sample ID
3.1	~ 2	600	75	20.23
7.8	~ 2	600	75	20.21
9.5	~ 2	600	75	20.22
3.0	3.0	480	75	20.16
7.6	2.8	480	75	20.14
10.5	3.4	480	75	20.15

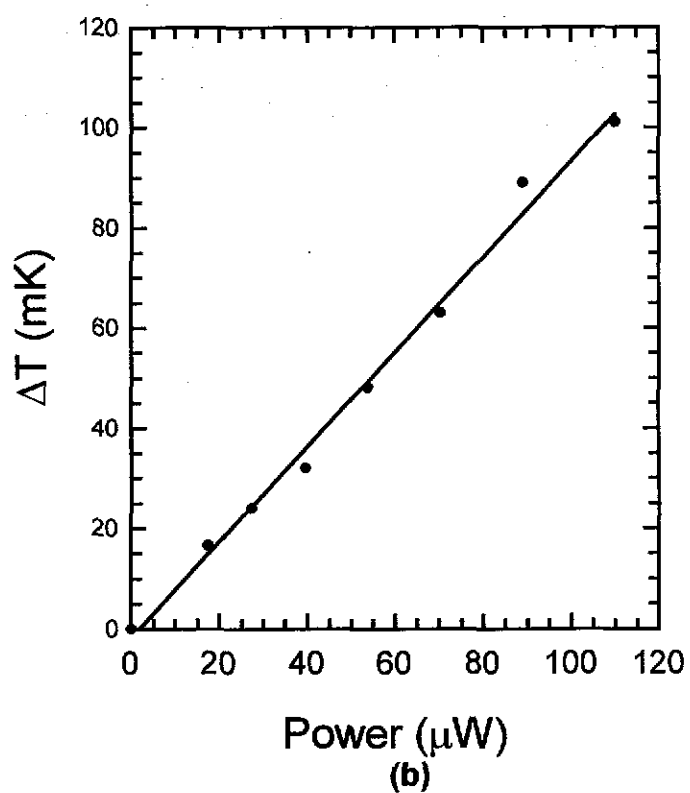
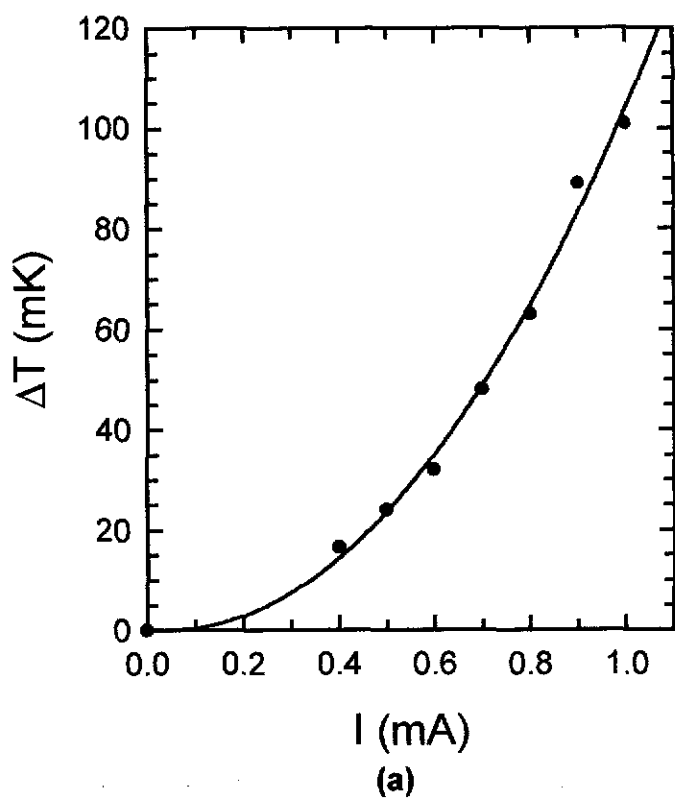


Figure 5.5: Temperature gradient ∇T vs. top heater current I at 1.5 K for the 2DHG sample 20.15 (a). Temperature gradient vs. heater power in (b).

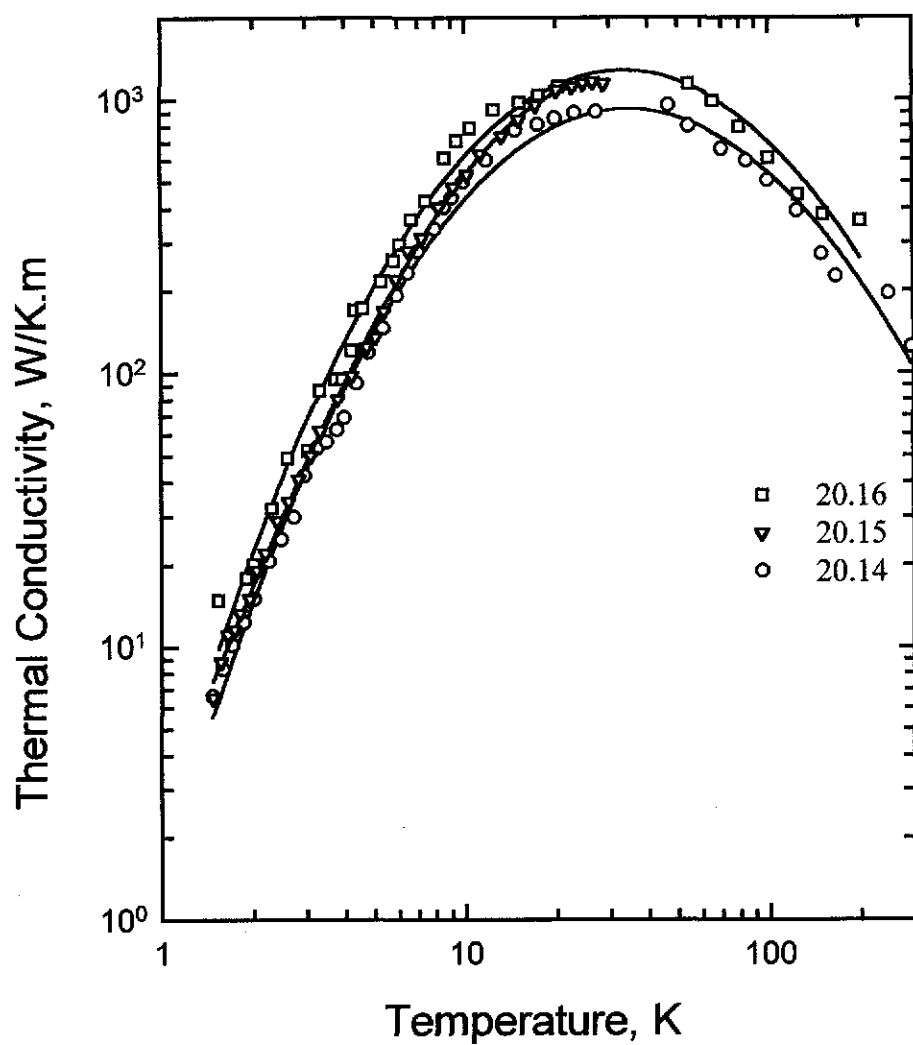


Figure 5.6: Thermal conductivity results for the Si- δ - $\langle B \rangle$ doped structures with the substrate doping concentrations: $\square$ $1.7 \times 10^{15} \text{ cm}^{-3}$, $\circ$ $2.7 \times 10^{15} \text{ cm}^{-3}$, and ∇ $2.1 \times 10^{15} \text{ cm}^{-3}$.

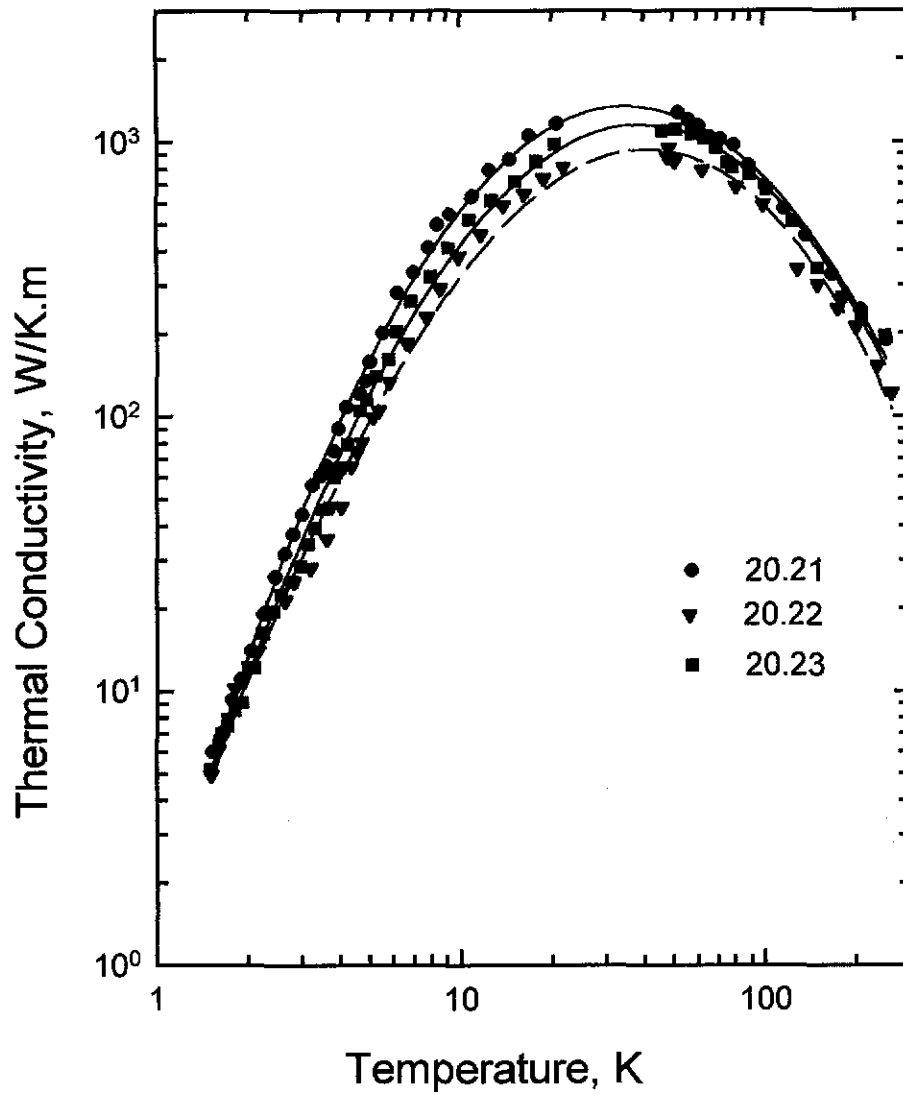


Figure 5.7: Thermal conductivity results for the Si-δ-<Sb> doped structures with the substrate doping concentrations: ■ $6 \times 10^{15} \text{ cm}^{-3}$, ● $4.9 \times 10^{15} \text{ cm}^{-3}$, and ▼ $7.1 \times 10^{15} \text{ cm}^{-3}$.

Thermal conductivity of the samples have been measured in the temperature range 1.5-250 K. In general, the thermal conductivity of single crystal silicon exhibits a temperature dependence, characteristics of single crystal dielectric materials. For the purest silicon samples, the thermal conductivity goes through a maximum at a temperature of about 22 K. Above this temperature, the conductivity falls as the phonon mean free path is reduced by phonon-phonon scattering processes. At temperatures below the maximum, the absolute value of the conductivity is highly dependent on the sample but, in broad terms, it falls with a temperature dependence close to that of the specific heat of the lattice (T^3) (seen in **Figure 5.8**).

Table 5.3: The parameters for the studied Si delta-B and delta-Sb doped samples

Delta channel type and resistivity ρ (k Ω / $\square$) @4.2 K	$k_F l$ Fermi wave vector times mean free path	Substrate type and resistivity ρ_s (Ω -cm) @300 K	Substrate doping con. (10^{15} cm $^{-3}$)	Substrate phonon mean free path l_p (mm) 1.5 K/4.2 K
n /6.19	3.0	p^+ /2.11	6.0	1.53/1.06
n /1.53	12.0	p^+ /3.50	4.9	1.69/1.11
n /1.17	15.6	p^+ /1.86	7.1	1.44/0.71
p /4.76	2.7	n^- /2.51	1.7	3.0/1.62
p /1.89	5.0	n^- /1.73	2.7	1.9/1.20
p /1.43	12.8	n^- /2.00	2.1	2.1/1.38

The thermal conductivity of silicon has been measured over a wide temperature range and a variety of samples by many workers. The thermal conductivity data is shown for doped silicon (taken from EMIS Datareviews No:4 by M.N. Wybourne (1988)) (**Figure: 5.9**). In the temperature range up to 200 K, details of the temperature dependence of the thermal conductivity together with the position and magnitude of the conductivity maximum, are sensitive to the size, perfection, doping level and type, orientation and surface quality of the sample.

5.5 Phonon mean free path calculations

The phonon boundary scattering is most important at low temperatures, where the mean free paths of phonons are longest. Boundary scattering is very significant at room temperature in thin silicon layers. The thermal conductivity of the entire structure may be used to deduce C_v in Eq. (2-16) using the values $v_t = 5.331 \times 10^3 \text{ m s}^{-1}$ and $v_l = 8.861 \times 10^3 \text{ m s}^{-1}$, for acoustic transverse and longitudinal modes in Si, respectively. We estimate v_s to be $5.896 \times 10^3 \text{ ms}^{-1}$. The phonon specific heat C_v in the Debye approximation for the three acoustic branches have been used for the calculation of l_p as in Eq. (2-9).

Phonon mean free paths have been calculated from the thermal conductivity results for delta boron doped 2DHG samples (shown in **Figure 5.10**) and delta antimony doped 2DEG samples (given in **Figure 5.11**). These results show that there are small differences at low temperatures, but at high

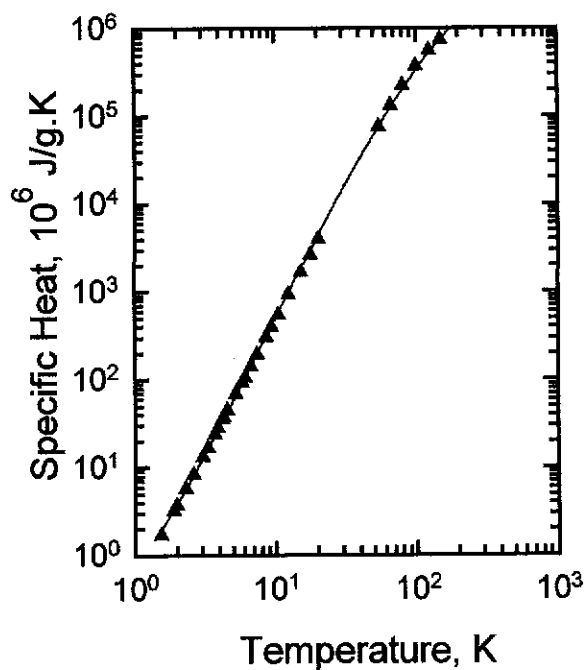


Figure 5.8: Specific heat vs. temperature for the Si/δ-⟨B⟩/Si doped sample 20.16.

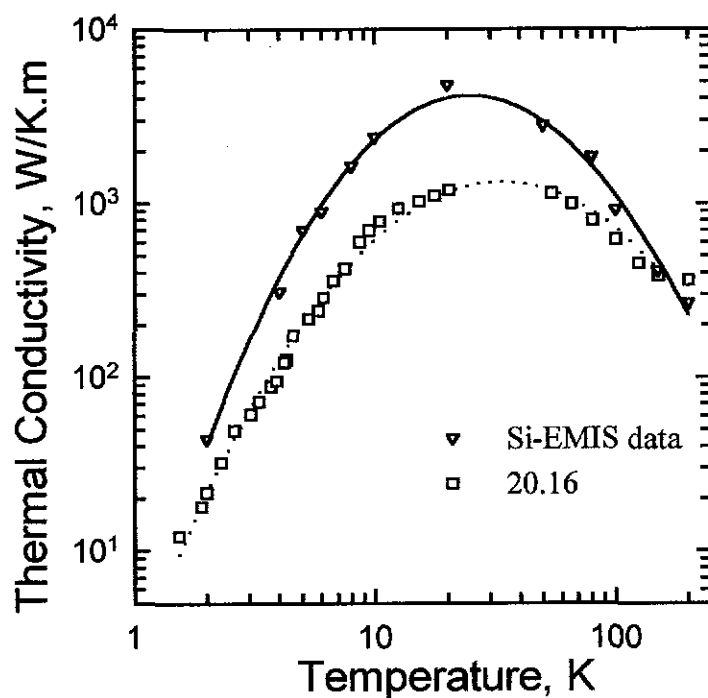


Figure 5.9: Experimental thermal conductivity results for the Si/δ-⟨B⟩/Si doped sample 20.16 with compared EMIS Data book data of Si.

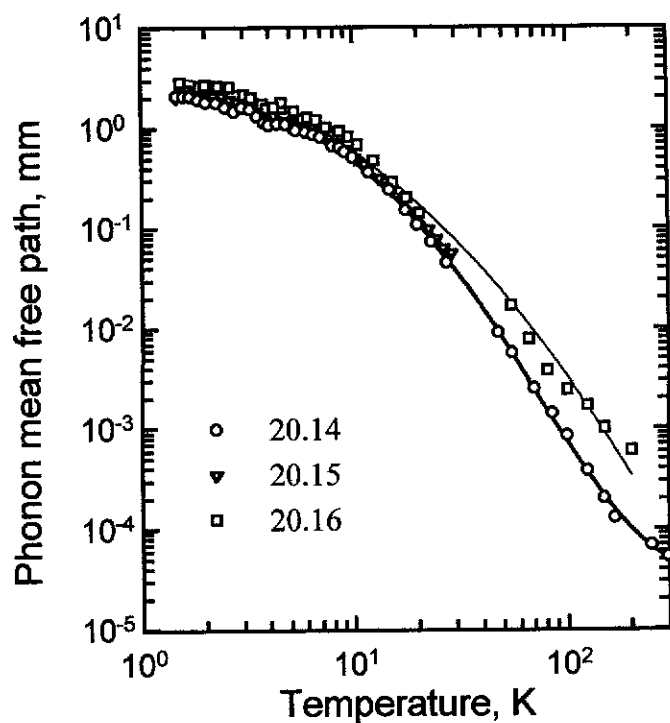


Figure 5.10: Experimental phonon mean free path measurements for the Si/δ-⟨B⟩/Si doped three samples.

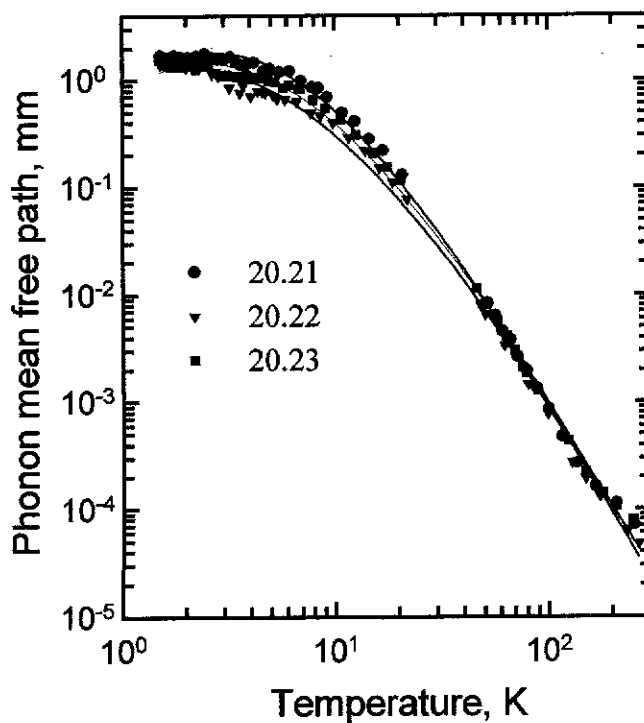


Figure 5.11: Experimental phonon mean free path measurements for the Si/δ-⟨Sb⟩/Si doped three samples.

temperatures, generally the same values have been obtained. For all the samples, substrate resistivities have been measured by a four point probe method (Table 5.3) using a 100 μA current. Doping concentrations were determined from p -Si and n -Si substrate resistivity. Higher resistance substrate has less doping concentration. More doping concentration causes less thermal conductivity or phonon mean free path. Generally, we can see this trend in Table 5.3 and in the phonon mean free path graphs.

5.6 Thermopower results

In this work, the first measurements of the thermopower p -type and n -type delta-doped Si are presented. At these low temperatures, the total thermoelectric power in zero magnetic field corresponds with the expected behaviour. The thermoelectric power, S , was deduced by a differential method, establishing that ΔV was linearly proportional to ΔT by taking the slope. Figure 5.12 has been obtained at 1.5 K for the delta B doped sample 20.15.

5.6.1 Diffusion thermopower

Measurement of thermopower in the temperature range 1.4 K to 30 K is shown in Figure 5.13. According to (2-24) $S_d \ll S_g$ in this temperature range is some tens of $\mu\text{V/K}$. As one can see, the presence of the smallest influence of diffusion term in the measured thermopower signal is due to changes in the slope from positive to negative with $S_d/\lambda_L \propto T^2$. This is observed only in the case of

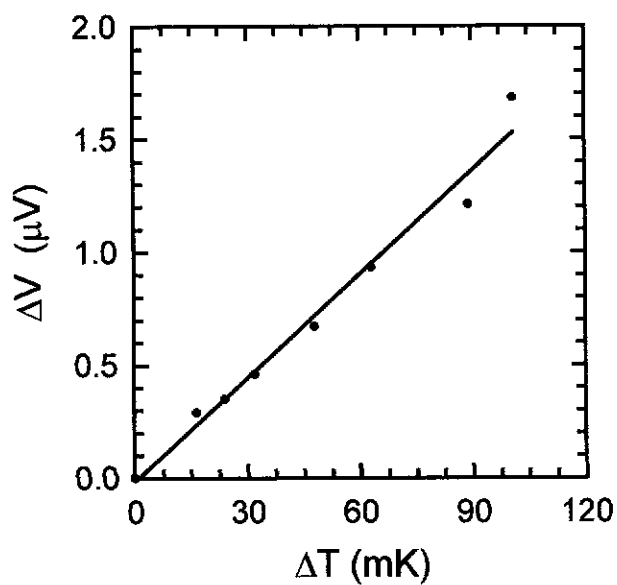


Figure 5.12: Experimental voltage gradient vs. temperature gradient of thermopower measurements for p-type delta B doped sample at 1.5 K with $1 \times 10^{14} \text{ cm}^{-2}$ carrier density.

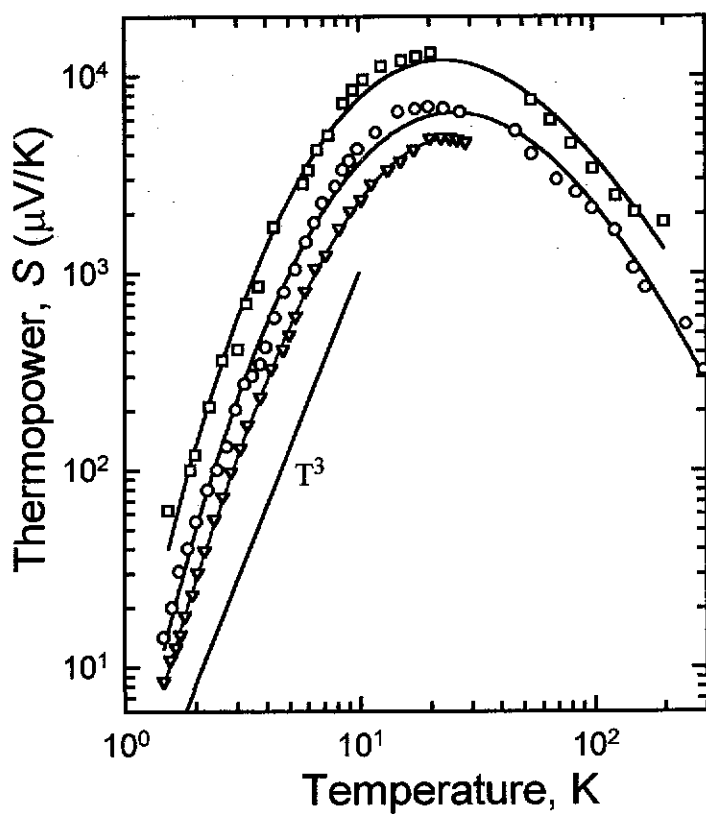


Figure 5.13: Temperature dependence of thermoelectric power at low temperatures for δ - Si doped samples: □ 20.16, ○ 20.14, ▼ 20.15 with $3 \times 10^{13} \text{ cm}^{-2}$, $7.6 \times 10^{13} \text{ cm}^{-2}$ and $10.5 \times 10^{13} \text{ cm}^{-2}$ sheet densities, respectively.

our $3.1 \times 10^{13} \text{ cm}^{-2}$ sheet density (n-type) measured sample (see Figure 5.18a) at the lowest temperatures. The $S(T)$ maxima, in the range from 2 mV/K and 14 mV/K near 25 K, are caused by phonon drag and are very similar in order of magnitude and temperature to those seen in SiGe/(100)Si 2DHG with much smaller p_s .

Since the diffusion component was never fully developed in the results for the 2DHG systems, it was hoped that the greater sheet density of the delta layer systems would yield interesting diffusion thermopower results for a two dimensional system at the higher temperature regime. In fact, Fletcher *et al.*, (1994) report this on a low mobility 2DEG with a very high Fermi temperature. This delta layer system, however, consisted of a single Si δ -layer grown within a confining 10 nm GaAs well which modified the energy levels to populate mostly just the ground state energy level.

5.6.2 Phonon drag thermopower

The samples we have investigated in the present work have a mobility μ_H of about 20-50 cm^2/Vs , which is more than an order of magnitude lower than that used in earlier studies (Fletcher *et al.*, 1994) and can provide a direct test of whether the phonon drag is reduced by a lower mobility. Gerleman (1998) reported experimental thermopower results for similar structures above 3 K and no theoretical calculations for thermoelectric properties were reported before for delta-doped structures with multi-subband occupation by free carriers. These results, together with those of (Fletcher *et al.*, 1994), should put to rest any

suggestion that phonon-drag is small for the low carrier mobility (20-50 cm²/V.s in the present case). The magnitude of S increases as n_s or p_s is reduced in the temperature range 1.4 K < T < 25 K.

The thermoelectric power of the two dimensional hole (2DHG) delta-B (Figure 5.13) and electron gases (2DEG) delta-Sb doped Si structures (Figure 5.14 and Figure 5.15) were measured for the first time. The temperature range was 1.4 K to 300 K, and carrier sheet densities were in the range 0.3 to 1.05 × 10¹⁴ cm⁻². The thermopower was dominated by the phonon drag contribution.

The general shape of the thermopower curves is fairly well explained. The large, wide peak at low temperatures is ascribable to phonon drag due to its, 1/ n_s , dependence. The sign of the thermal voltage also correctly reflected the nature of the 2D gas within, i.e. positive for holes and negative for electrons. The change from positive to negative thermopower for the Sb delta layers indicates a change from substrate dominated thermopower at high temperatures to 2DEG dominated at low temperatures.

The dashed lines in Figure 5.16 (a) and 5.16 (b) show the values of S calculated for one of the delta B-doped Si sample with $p_s = 3 \times 10^{13}$ cm⁻² (Agan *et al.*, 2000b). A screened potential ($\Xi_{\text{eff}} = 18$ eV) is used in the first curve, Figure 5.16 (a), and an unscreened potential ($\Xi_{\text{eff}} = 12$ eV) in the second, Figure 5.16 (b). The unscreened scattering potential seems to give a better fit to the experimental data, for it use a realistic value of Ξ_{eff} (Zavaritskii and Kvon, 1983). This result is consistent with measurements of hot carrier energy loss rates in the SiGe 2DHG (Ansari pour *et al.*, 2000) which also suggest that the hot-acoustic

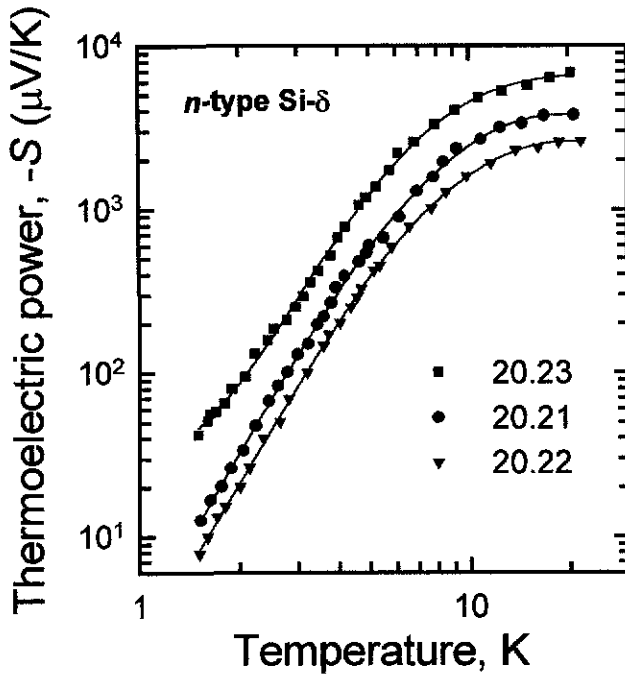


Figure 5.14: Temperature dependence of thermoelectric power at low temperatures for Si-δ-<Sb> doped samples: with (20.23) $3.1 \times 10^{13} \text{ cm}^{-2}$, (20.21) $7.8 \times 10^{13} \text{ cm}^{-2}$ and (20.22) $9.5 \times 10^{13} \text{ cm}^{-2}$ sheet densities.

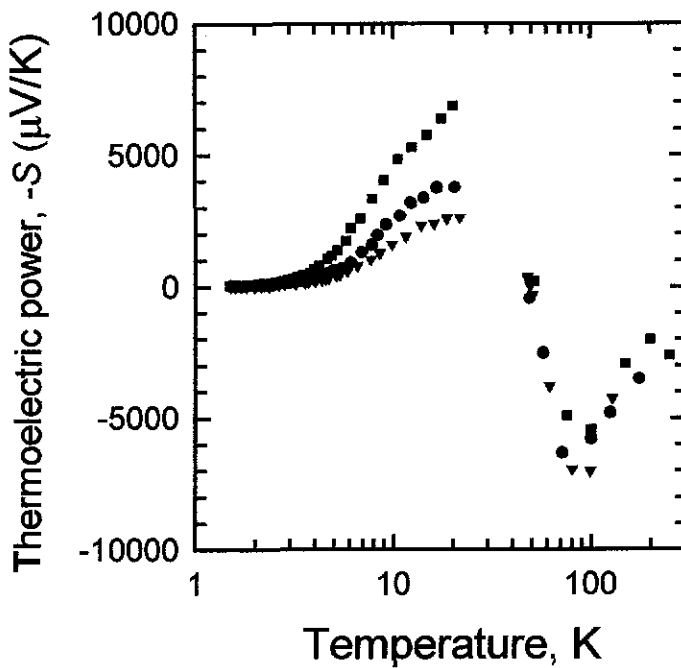


Figure 5.15: Temperature dependence of thermoelectric power in the temperature range 1.5 - 300 K for same Si-δ-<Sb> doped samples.

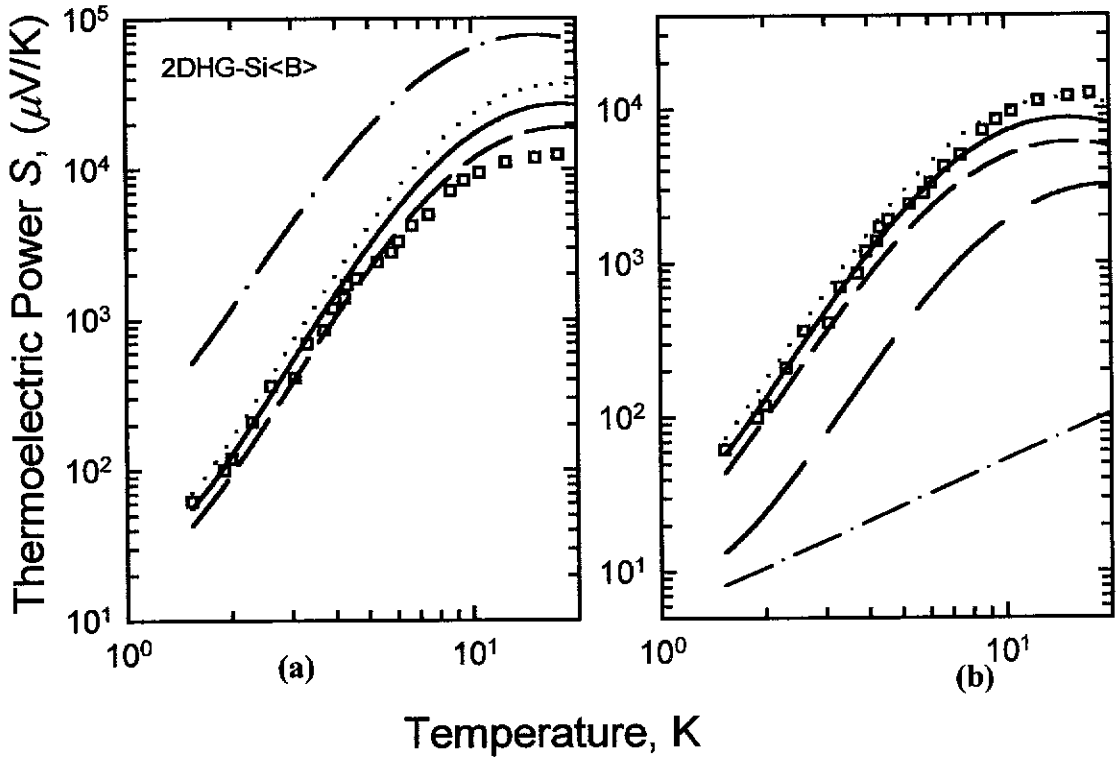


Figure 5.16: Temperature dependent thermopower: Experimental results ($\square$) and theoretical calculations including phonon-drag with screened and unscreened hole-phonon interaction, for a 2DHG delta B doped sample with $3.0 \times 10^{13} \text{ cm}^{-2}$ sheet carrier density. The effective mass is $m^* = 0.9 m_0$. In (a), screened deformation potentials are 15 eV (dashed line), 18 eV (solid line), 21 eV (dotted line). Also shown is the theoretical unscreened hole phonon interaction for deformation potential of 18 eV (dashed dot line). In (b), the deformation potentials of 12 eV screened (long dashed line). Theoretical unscreened hole-phonon interactions are shown for $\Xi = 10$ eV (small dashed line), 12 eV (solid line) and 14 eV (dotted line). Dashed dot line gives the diffusion thermopower S_d ($p = 1$).

phonon interaction is best treated as unscreened. The 2DEG sample (Figure 5.17) ($g_v=2$) has the same carrier density and shows the screened calculation ($\Xi_{\text{eff}}=20$ eV), Figure 5.17 (a), and an unscreened potential ($\Xi_{\text{eff}}=10$ eV) in the second, Figure 5.17 (b). We can see again (as for $\delta\text{-B>Si}$ sample) that screened deformation potential values are unrealistically large. In the literature this is given as 7.3 eV for an electron gas on (001) Si, and 12.3 eV for a hole gas on (111) Si (Zavaritskii, 1984). The effective masses are used $0.9 m_0$ for 2DHG and $0.19 m_0$ 2DEG. The pronounced discrepancy between experiment and theory at $T > 10$ K in either case can be understood on the basis of (i) the different average phonon mean free paths involved in thermal conductivity and thermopower (Gallagher and Butcher, 1992) and (ii) the existence of 3D conduction through the substrate at $T > 25$ K.

We believe that the intersubband scattering is large in the samples studied (momentum relaxation time, τ , is quite low $\sim 10^{-14}$ s and $\Gamma_\tau = \hbar/2\tau$, level broadening is 60-150 meV). The nature of δ -layers in which the impurity atoms generating the quantum potential well are themselves the factors of intensive impurity-induced scattering. Under the condition of strong intersubband scattering, the subbands are smeared. We may assume that the system behaves as if it contains one “effective” subband. A similar conclusion is reached for multivalley systems if the rate of intervalley scattering is high enough (Agan *et al.*, 2000c).

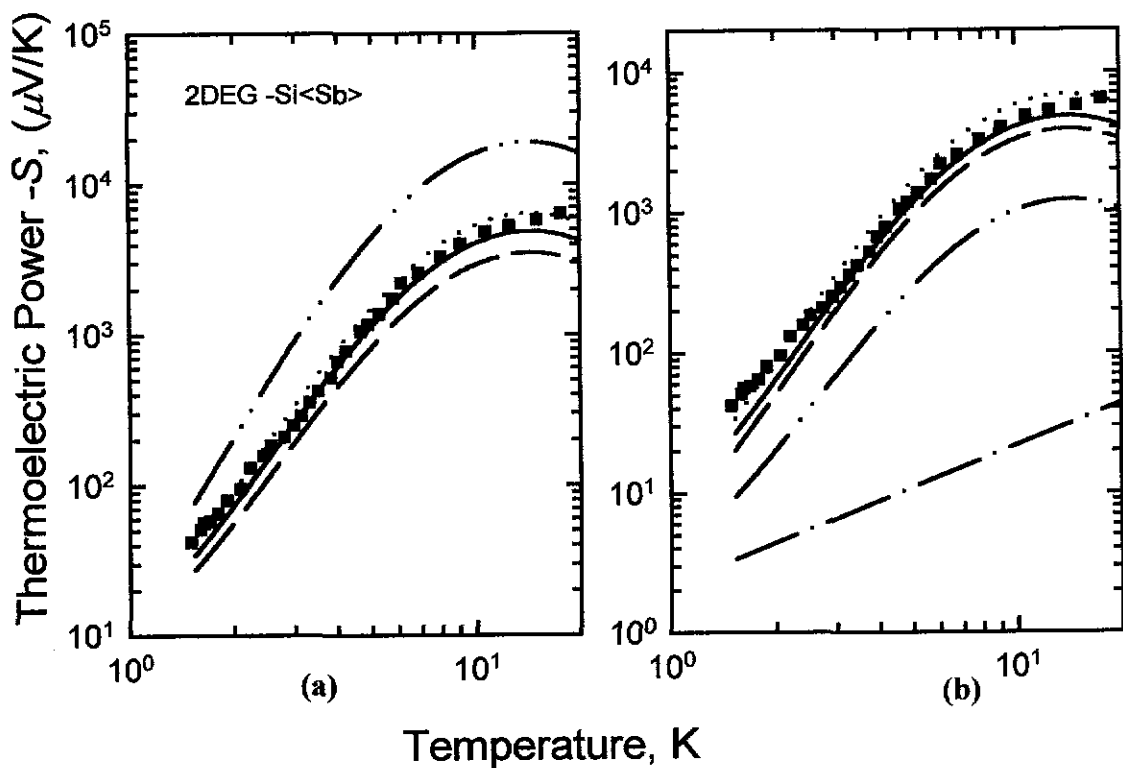


Figure 5.17: Temperature dependent thermopower: Experimental results (■) and theoretical calculations (lines) including phonon-drag with screened and unscreened electron-phonon interaction, for a 2DEG delta Sb doped sample with $3.1 \times 10^{13} \text{ cm}^{-2}$ sheet carrier density. In (a), the theoretical thermopower is shown for screened deformation potential values of 17 eV (small dashed line), 20 eV (solid line) and 23 eV (dotted line). The dashed dot-dot line shows theoretical 20 eV unscreened deformation potential interaction. In (b), unscreened interaction which deformation potential of 9 eV (small dashed line), 10 eV (solid line) and 11 eV (dotted line). The dashed dot-dot line shows 10 eV screened deformation potential interaction. Dashed dot line gives the diffusion thermopower S_d ($p=1$).

5.7 Kohn anomaly of thermopower in Si/ δ -B and δ -Sb layers

As seen from (Figure 5.18) the ratio S/λ_L in the low temperature limit ($\lambda_L \propto T^3$, as is observed in Figure 5.6) is sensitive to the strength of carrier-phonon interaction and defines the shape of $F(T, n_s)$. The single maximum in the range 1.5-30 K is seen for every investigated sample. We believe this corresponds to resonant phonon absorption (Kohn anomaly). According with Eq. (2-21) position of discussed maxima $T^{KA} \propto (p_s/g_v)^{0.5}$, it roughly scales with the sheet density as expected and with the value of valley degeneracy g_v , which explains the difference between n -type and p -type samples. The existence of one broad maximum for multi subband occupied samples can be explained by the resolvable limit for observation of multi maxima behaviour, but needs more theoretical work for quantitative interpretation.

5.8 Quantum interference effects in the case of metal-type conductivity

The metallic conductivity of δ -layers (samples 20.22, 20.21 and 20.23) exhibits manifestations of WL (Abrahams *et al.*, 1979) and EEI (Altshuler, Aronov and Lee, 1980 and Lee and Ramakrishnan, 1985) effects. In a previous paper, Matthey, *et al.*, (1992b) argued that the electrical properties in the “metallic” regime could be adequately described by assuming occupancy of a single subband, due to the fact that intersubband scattering effects were relatively strong. These effects occur in disordered systems under the condition

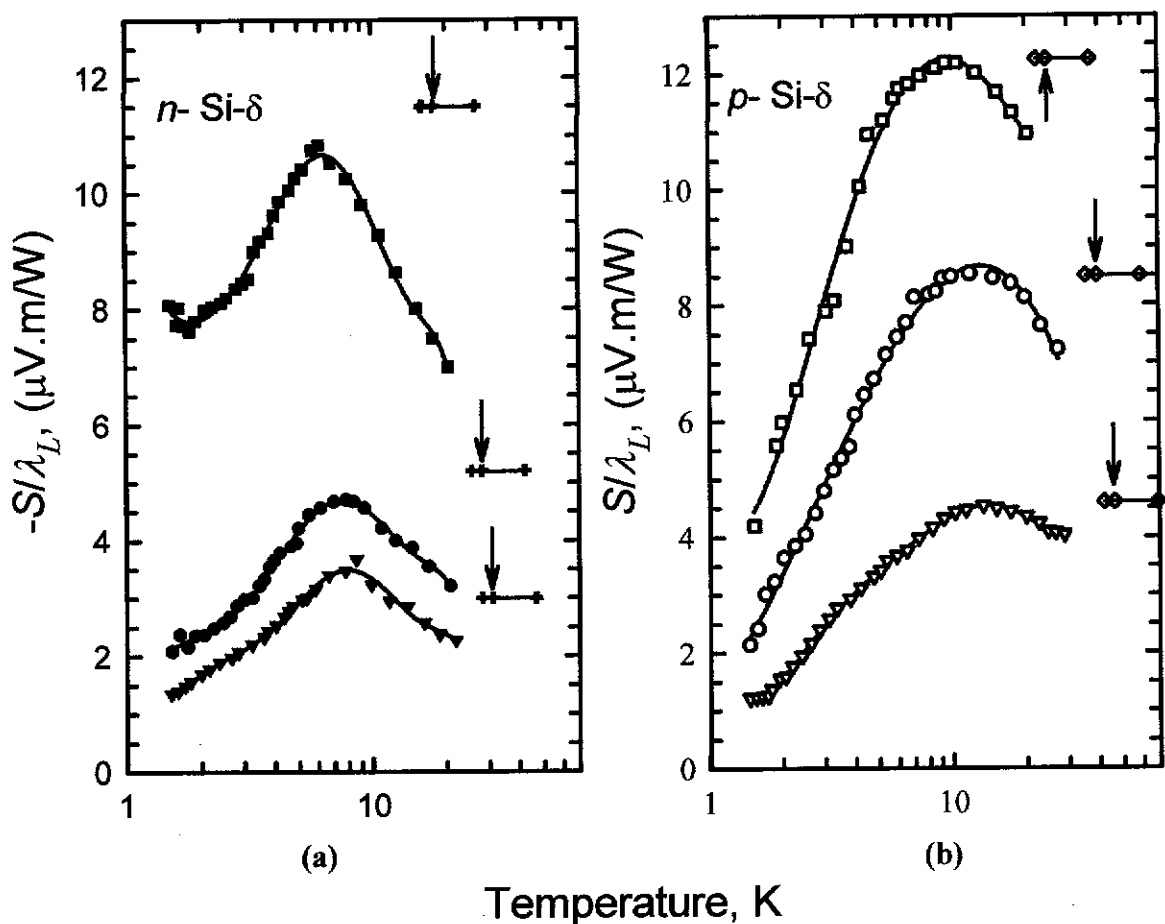


Figure 5.18: The ratio of the thermopower S to thermal conductivity λ_L as a function of temperature for $\text{Si-}\delta\text{-}\langle\text{Sb}\rangle$ and $\text{Si-}\delta\text{-}\langle\text{B}\rangle$ doped samples with the parameters given in the captions to Figures 5.13 and 5.14. For n-type sample crosses give estimated Kohn temperatures T^{KA} for v_b , v_l and v_s (arrows) taking valley degeneracy $g_v=2$. p-type sample estimated values have been given ($g_v=1$) as open diamonds. Although there is a discrepancy between absolute theoretical and experimental values of the Kohn anomaly temperature T^{KA} , where expected sheet density dependence is clearly observed in the experimental data.

of strong elastic scattering of electrons: they arise from interference and require quantum corrections to the conductivity, which results in the resistance being dependent on both temperature and magnetic field.

Plotting $1/S$ against carrier sheet densities shows that for metallic densities the points lie on straight line which intercepts the axis near density $n_{MIT} \approx 10^{13} \text{ cm}^{-2}$, which corresponds to the transition from weakly to strongly localised conductivity regimes. One can see that S_g scales with inverse sheet carrier densities are in extended states. **Figure 5.19** show the $1/S$ vs n_s relationships for the B delta layers. The value corresponds well with the results of Matthey *et al.*, (1992b) and van Gorkum, Nakagawa and Shiraki, (1989) for the metal insulator transition in these systems.

In uniformly doped Si:B, the onset of metallic behaviour occurs at an average impurity separation of 3.5 nm (Chroboczek *et al.*, 1984), whereas the average impurity separation in the δ -layer is $2.2 \pm 0.1 \text{ nm}$ as deduced from the peak concentration of the SIMS profile ($2.2 \times 10^{19} \text{ cm}^{-3}$), is itself an underestimate. Similar behaviour has been observed in Sb (van Gorkum, Nakagawa and Shiraki, 1989) and As δ -layers in Si (Denhoff *et al.*, 1989).

For both the boron and antimony delta layer systems, there is similar behaviour as regards phonon drag. The evidence for phonon drag is strong in the more heavily doped samples with a dependency on temperature of approximately T^3 . Also, for all samples there is a clear inverse relationship of thermopower on sheet carrier density. For lightly doped samples that are near

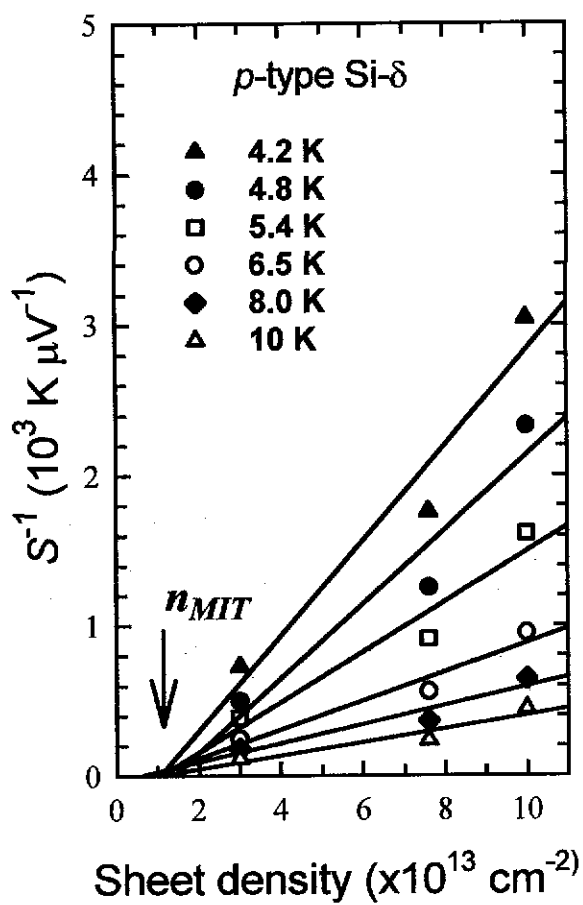


Figure 5.19: Inverse thermopower as a function of carrier density for $\delta < B >$ doped Si structures in the temperature range 4.2-10 K. The metal-insulator transition occurs at $1 \times 10^{13} \text{ cm}^{-2}$ carrier sheet density (n_{MIT}).

the transition density, it is possible that the mixed state of conduction could distort the temperature dependency of the thermopower.

5.9 Parallel transport in Si/ δ and <Sb> layers

The thermopower characteristics of the Sb samples show the transition from 2DEG dominated transport characteristics to 3D substrate domination. The thermopower shows the changeover from 2D (electron) conduction to 3D (substrate hole) conduction evidenced for the transition point. The contact material of the samples is p-type Aluminium, which has been seen to contact well with the degenerate 2DEG of the Sb channels (Biswas *et al.*, 1993; Whall, 1992). However, when the 2DEG loses degeneracy and bulk 3D parallel effects become prevalent there is also good contact, with the Al contact material, to the p-type substrate.

The boron delta layers, by the nature of the contacts, show a different characteristic. The Al contacts isolate the n- substrate from electrical measurement at all temperatures and hence the δ -layer is measured in isolation throughout the full temperature range.

5.10 Conclusions and discussions

The study of δ -layers in silicon becomes interesting for device applications. Delta-doped semiconductors offer new opportunities for the study of the electrical conduction in low-dimensional systems. Delta layers also make

possible the realisation of low-dimensional and other novel device structures in a single semiconductor, and could well find a role in future integrated-circuit technology (Whall, 1992).

The studies of the electrical properties of Si single crystals with a $\delta\text{-Sb}$ -layer of various sheet concentrations N_D of Sb atoms ($5 \cdot 10^{12} - 3 \cdot 10^{14} \text{ cm}^{-2}$) have provided detailed information about the low temperature features of the electron transport in this system. The findings are as follows.

1. At n_s below $\sim 3 \times 10^{13} \text{ cm}^{-2}$ a metal-insulator transition occurs, which is accompanied by a change from metal-type conductivity of $\delta\text{-Sb}$ -layer to hopping conductivity in a 2D system.
2. As the temperature is increased, the impurity conduction in the δ -layer changes to a higher conductivity in the Si crystal due to activation of the electrons to the conduction band. The change of impurity conductivity to band conductivity with increasing n_s occurs at progressively higher temperatures.

In the temperature range 1-10 K, further interesting effects that lead to a deviation from the T^3 behaviour were predicted and observed for the thermal conductivity experiments.

The phonon drag was clearly demonstrated in both Sb and B doped channels. It has been shown, however, that the magnitude of the drag thermopower is strongly influenced by a loss of degeneracy as the donor density approached that of the metal insulator transition density. The dominance of phonon drag on the thermopower of these systems unfortunately masks, and

have effects that might be due to weak localisation and carrier-carrier interactions in the zero field thermopower of these samples.

The modulation boron doped Si/Si_{0.93}Ge_{0.07} 2DHG sample (in Chapter 4) (32.12) has a 460-510 times higher mobility than those of the boron delta doped samples 20.14 and 20.16 at a temperature of 4.2 K. But the thermopower of 32.12 is 1.5-3.0 less than those of 20.14 and 20.16 at 25 K. These results, together with those of (Fletcher *et al.*, 1994), should put to rest any suggestion (Ruf *et al.*, 1989) that phonon-drag is small for 2DHGs of low carrier mobility. On the other hand, the sheet density of sample 32.12 is 375-875 times less than those of 20.16 and 20.14.

The maximum value of the thermopower signal for all samples is observed to be at ~25 K. Comparing sample 20.16 with 20.14 both of which have delta boron doped layers we can say that the former has a sheet carrier density which is approximately half that of the latter, but its thermopower signal is twice that of 20.14. These experimental results correspond well with theory (Cantrell-Butcher theory).

The low temperature thermoelectric power of low mobility and very high density 2DEG and 2DHG of delta antimony and boron doped Si structures were measured for the first time and were found to be dominated by phonon drag for the temperature range 1.4-30 K. In the range 6-14 K, for all the samples, we observed a maximum in the ratio of the thermopower to thermal conductivity which corresponds to resonant phonon absorption across the “most effective” Fermi circle (Kohn anomaly). The temperature dependence of the thermopower

was described most accurately by an unscreened potential when calculating the phonon-drag for 2DHG and 2DEG.

Chapter Six

Conclusions

and

Suggestions for Further Work

Sheet density and Hall mobility as a function of temperatures were measured in normal and inverted modulation doped structures. Low temperature magnetotransport measurements (down to 0.33 K and at magnetic fields up to 12 T) were carried out on one inverted sample. The hole effective mass was extracted from the temperature dependence of Subnikov de Haas oscillations in 2DHG resistance.

Experimental data on thermopower in two dimensional hole gases (2DHGs) confined in strained Si/Si_{1-x}Ge_x structures fabricated at Warwick, were explained successfully by using the conventional phonon drag formalism, when $B=0$. Our concern, in this thesis, was to understand the thermoelectric transport properties of two dimensional hole and electron gases in semiconductor devices. When electrons are confined to move in less than three directions, they exhibit a number of fascinating properties, and because of that, low dimensional structures

have attracted a great deal of theoretical and technological interest in the last two decades.

The experimental equipment and procedures were very successful and provided results of a high quality. This was achieved by a careful study in the field of low temperature thermal measurements. Although the apparatus used was designed according to the requirements of this specific work, it is useful for a variety of thermal and electrical work. The cryostat was designed to achieve a highly insulating sample space vacuum, to enable the study of the large cooling power of the samples and the wide range of temperatures that could be attained (1.5 – 300 K).

The details for the B and Sb layers differ, however, and this is due to the method used to contact the δ -layers. For the B layers, the Al contacts isolate the n^- substrate at all temperatures and the properties of the B layer are measured at all temperatures. A large enhancement to the thermopower due to phonon drag may be seen in the temperature range 1.5-80 K. At the upper end of this range, however, the Boron layer is suspected to have lost its 2D nature (Mattey *et al.*, 1992) and so one is not actually studying a 2DHG any longer.

As the doping density of the δ -layers approaches the transition from degenerate conduction to insulator like behaviour, the thermopower (phonon drag dominated) is seen to increase strongly, breaking the linearity of the $1/S$ versus sheet density plots. The convergence of these plots to a particular sheet carrier density is confirmed to be a determination of metal insulator transition in these systems. This is supported by the evidence of previous workers (Mattey *et*

al., 1992b; van Gorkum, Nakagawa and Shiraki, 1989). However, the effect of parallel conduction at low temperatures (<20 K) is usually negligible.

The δ -layer systems also enabled an new study on parallel conduction, in particular on the Sb layers. A changeover from negative to positive thermopower above 50 K with the Sb samples indicates a change from the dominance of the 2DEG to the *p*-type substrate at this temperature. This result ties in well with the work of Kashirin *et al.*, (1996). For the B doped systems the δ -layer is contacted at all temperatures. But it is not certain what influence the substrate has at higher temperatures as the loss of degeneracy of the δ -layer causes the resistivity of the two parallel paths to become more similar.

We paid particular attention to thermopower at temperatures up to room temperature in a zero magnetic field. The phonon-drag calculations were based on Cantrell-Butcher (CB) theory. Some improvement was made by considering the temperature dependence of screening and unscreening, the phonon mean free path and the effect of thermal broadening of the Fermi function. It has been confirmed that the existing phonon drag theory is successful in explaining the main features of the thermopower data. The data that were obtained generally corresponded well with the theory. However, no interface acoustic phonons exist in the heterojunction and the physical origin of the change of the deformation potential is not clear. Nevertheless, a modification of the deformation potential value in either system is directly reflected in the correspondence between theory and experiment. In Si the lattice anisotropy in the electron-phonon interaction has been regarded as small, and instead of considering each direction of the

phonon wavevector $\mathbf{Q}$ separately in calculating the transition rate, as it has been done by Herring and Vogt (1956), an implicit averaging over the azimuthal angle of $\mathbf{Q}$ was adopted. Proper consideration of the phonon anisotropy would broaden the phonon distribution and further enhance the electron-phonon interaction at high temperatures and low electron densities.

A good understanding of the zero-magnetic field thermopower is also useful for the non-zero magnetic field case in the quantum limit. An interesting problem is the calculation of phonon drag contribution to transport coefficients in systems where quantum transport takes place. Calculations and measurements of thermotransport in these systems may prove challenging in the near-future.

At temperatures higher than 60 K, the phonon drag decreases dramatically due to an abrupt decrease in the phonon mean free paths, as the diffusion contribution becomes dominant. The calculations of the diffusion and phonon drag contributions to the thermoelectric coefficients have been made by using the theoretical formalism presented in Chapter 2. In the diffusion regime, the theory predicts very well the thermopower behaviour for all the temperatures and magnetic fields investigated. Moreover, for the calculation of the phonon drag thermopower in zero field, S , we initially used the phonon mean free paths derived from the thermal conductivity measurements. The next theoretical step would be to develop the microscopic theory further so as to introduce realistic dependencies of the mean free paths on the phonon wave vector.

The phonon momentum transferred to the holes was worked out from the theory of Zavaritsky (1984). The peaks observed in S/λ_L as a function of T were qualitatively explained in enhancement terms of the hole-phonon interaction

The work described in this thesis has raised several questions which suggest interesting areas for future investigation. More theoretical work is needed to investigate the effects of the multisubband conduction and relatively high degree of disorder. The critical sheet density ($\sim 1 \times 10^{13} \text{ cm}^{-2}$) for the metal-insulator transition seems to be larger than the equivalent bulk value in the present samples and should be the subject of further experimental and theoretical investigation.

Experiments at lower temperatures (below 1.5 K) are needed to get more information and to investigate the diffusion thermopower contribution. More 2DEG Si/SiGe heterostructures could be measured to obtain a more varied sheet density dependence of thermopower. As a future work, the thermopower of one dimensional quantum wires in Si-based structures could be measured. Experiments could also be extended to measure magnetothermopower in Si/SiGe heterostructures and delta doped layers in Si.

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