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ELECTRICAL PROPERTIES OF GaAs$_{1-x}$P$_x$

DISSEMINATION

Presented in Partial Fulfillment of the Requirements for the Degree Doctor of Philosophy in the Graduate School of The Ohio State University

by

Hamed S. Abdel-Hameed Bayoumi,
B.S. E.E., M.E.E.

* * * * * * *

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1970

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<td>a</td>
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<td>one of Seitz magnetoresistance coefficients, $=\frac{\rho_{1122}}{\rho_0}$</td>
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<td>B</td>
<td>magnetic field density</td>
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<td>c</td>
<td>one of Seitz magnetoresistance coefficients, $=\frac{2\rho_{1212}}{\rho_0}$</td>
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<td>d</td>
<td>one of Seitz magnetoresistance coefficients, $=\frac{\rho_{1111} - \rho_{1122} - 2\rho_{1212}}{\rho_0}$</td>
<td></td>
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<tr>
<td>D</td>
<td>number of energy minima or maxima symmetrically situated in the Brillouin zone.</td>
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<tr>
<td>e</td>
<td>magnitude of electronic charge.</td>
<td></td>
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<tr>
<td>e</td>
<td>the base of the natural system of logarithms</td>
<td></td>
</tr>
<tr>
<td>E</td>
<td>electron energy</td>
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<td>$E_g$</td>
<td>energy gap</td>
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<tr>
<td>$E_1$</td>
<td>width of the direct energy gap at the center of the Brillouin zone.</td>
<td></td>
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<td>$E_2$</td>
<td>width of the indirect energy gap at X relative to the valence band maximum at (000).</td>
<td></td>
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<td>$E_d$</td>
<td>the ground ionization energy of the electron.</td>
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<td>$E_c$</td>
<td>energy level of the conduction band lowest minimum.</td>
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<td>$E_1,E_2,E_k,E_T$</td>
<td>electric field components.</td>
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<tr>
<td>f</td>
<td>$= f(x,K,t)$, electron distribution function.</td>
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<tr>
<td>$f_0(E)$</td>
<td>Fermi-Dirac distribution function.</td>
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<td>$f_1$</td>
<td>first perturbation of the electron distribution $f_0(E)$.</td>
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\( F_{\alpha}(n), F_{\beta}(n) \)  
Fermi integrals.

\( h \)  
Planck's constant.

\( \hbar \)  
Planck's constant.

\( J_i \)  
component of the electric current density.

\( k \)  
Boltzmann's constant.

\( K \)  
electron wave vector.

\( K_t(\omega) \)  
dielectric constant of a material in an electric field of angular frequency \( \omega \).

\( K_G \)  
Kilogauss.

\((\lambda_1, \lambda_2, \lambda_3)\)  
direction cosines of the current density \( J \).

\( L(E) \)  
density of electronic states of energy \( E \).

\( m_0 \)  
free electron mass.

\( m^* \)  
effective mass of the electron.

\( m_d \)  
density-of-states effective mass.

\( m_{1d}, m_{1d}^* \)  
density-of-states effective mass of the \( (000) \) valley.

\( m_{2d}, m_{2d}^* \)  
density-of-states effective mass of the \( <100> \) conduction band spheroids.

\( m_c \)  
conductivity effective mass.

\( n \)  
electron concentration, \( \text{cm}^{-3} \)

\( n_1, n_2 \)  
density of electrons in the \( (000) \) and \( <100> \) valleys.

\( N_a \)  
acceptor concentration.

\( N_d \)  
density of donor impurities.

\( N_{di} \)  
density of ionized donors.

\( N_i \)  
total number of ionized impurities.
List of Symbols (continued)

\( p \)  
\( \text{ratio of electron concentrations, } \frac{n_1}{n_2} \).

\( q_i \)  
component of heat current density.

\( r \)  
1) orbital radius of an electron around its positive ion.
2) exponent which depends on the type of scattering in the expression \( \tau = \tau_0 x^r \).
3) Hall coefficient factor, \( \frac{\mu_H}{\mu_c} \).

\( \mathbf{r} \)  
position vector.

\( R(B) \)  
Hall coefficient at a magnetic field density \( B \).

\( R_s \)  
Hall coefficient in the limit of zero magnetic field.

\( R_s \)  
screening radius.

\( s \)  
distance away from an ionized impurity centre.

\( S \)  
reduced energy separation between the conduction band edges at \( \mathbf{X} \) and \( \Gamma \) points, \( \frac{\Delta E}{kT} \).

\( t \)  
time.

\( T \)  
temperature in \( ^\circ \text{K} \).

\( x \)  
mole fraction of phosphorus in \( \text{GaAs}_{1-x} \text{P}_x \).

\( x_0 \)  
mole fraction of phosphorus in \( \text{GaAs}_{1-x} \text{P}_x \) at which the conduction band minima are at the same energy level.

\( (x_1, x_2, x_3) \)  
rectangular coordinate system.

\( x \)  
\( \frac{E - E_c}{kT} \) for n-type semiconductor.

\( X \)  
the point of intersection of Brillouin zone boundary with a \( <100> \) axis.

\( \mathbf{v} \)  
velocity vector.

\( w \)  
ratio of electron mobilities, \( \frac{\mu}{\mu_2} \).

\( a_1, a_2 \)  
\( \frac{m_1}{m_0}, \frac{m_2}{m_0} \) respectively.

\( r \)  
the centre of Brillouin zone.

\( \delta_{ij} \)  
the three dimensional unit tensor.
List of Symbols (continued)

ε
angle defined in the text.

ΔE
the energy separation between the conduction band minima at Γ and X, ΔE = E₂ - E₁.

∇ₓ
gradient vector in the electron wave vector space.

εᵢⱼₖ
= 1 if i, j, k form a positive sequence of 1, 2, 3
= -1 if i, j, k form a negative sequence of 1, 2, 3
= 0 if it contains two equal indices.

εᵣ
reduced ionization energy,
= \frac{Eᵣ}{kT}.

ζ
Fermi potential.

η
reduced energy separation between the conduction band lowest minimum and the Fermi level
= \frac{ζ - Eₓ}{kT}.

(η₁, η₂, η₃)
direction cosines of the magnetic field density B.

θ
angle between magnetic field direction and the sample length.

θₓ(T)
Debye Characteristic temperature at a lattice temperature T.

μ, μₓ
conductivity mobility.

μᵧ
Hall mobility.

μ₁, μ₂
mobilities of electrons in (000) and <100> valleys, respectively.

ξ*
electrochemical field intensity.

ξ
electric field intensity.

ρᵢⱼ(B)
resistivity tensor at a magnetic field B.
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<th>Definition</th>
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<td>first resistivity tensor coefficient, $= \rho_{ij}(0)$, the resistivity tensor at zero magnetic field.</td>
</tr>
<tr>
<td>$\rho_o$</td>
<td>diagonal element of the resistivity tensor of a cubic crystal in the absence of magnetic field, $\rho_{ij} = \rho_o \delta_{ij}$.</td>
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<tr>
<td>$\Delta \rho \over \rho_o$</td>
<td>relative change in resistivity due to magnetoresistance.</td>
</tr>
<tr>
<td>$\sigma_{ij}(B)$</td>
<td>conductivity tensor at a magnetic field $B$.</td>
</tr>
<tr>
<td>$\sigma_{ij}$</td>
<td>first conductivity tensor coefficient, $= \sigma_{ij}(0)$, conductivity tensor at zero magnetic field.</td>
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<tr>
<td>$\sigma_o$</td>
<td>diagonal element of the conductivity tensor of a cubic crystal in the absence of magnetic field, $\sigma_{ij} = \sigma_o \delta_{ij}$.</td>
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<td>$\tau$</td>
<td>relaxation time.</td>
</tr>
<tr>
<td>$\tau_i$</td>
<td>relaxation time of ionized impurities scattering.</td>
</tr>
<tr>
<td>$\tau_o$</td>
<td>optical phonons scattering relaxation time.</td>
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<tr>
<td>$\phi$</td>
<td>angle defined in the text.</td>
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<tr>
<td>$\psi$</td>
<td>angle between sample length and the [100] axis.</td>
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<td>$\omega_o$</td>
<td>optical phonons angular frequency.</td>
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<td>$&lt;&gt;$</td>
<td>averaging process defined in Section 4.5.1.</td>
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ELECTRICAL PROPERTIES OF GaAs\textsubscript{\(1-x\)P\(x\)}

INTRODUCTION

Transport processes involving spatial motion of particles and the transfer of momentum and/or energy, are an important class of physical phenomena.

In semiconductors, especially, the study of electronic transport effects has afforded much valuable information about the materials.

In this dissertation, three transport phenomena were used to study the electrical properties of the Gallium Arsenide Phosphide crystal alloy \([\text{GaAs}_{1-x}\text{P}_x]\). These phenomena are:

1) Electrical conductivity or resistivity
2) Hall effect
3) Magnetoresistance effect.

Measurements were made at various temperatures and for different specimen orientation and material composition. From these data, information about the structure of the conduction band and the scattering mechanisms in the crystal were obtained.

GaAs\textsubscript{\(1-x\)P\(x\)} is an important alloy because of its possible use in injection lasers of different designable output wavelengths. Its technology is still far behind that of GaAs as regards to crystal preparation and the understanding of transport properties and band structure. Most of the GaAs\textsubscript{\(1-x\)P\(x\)} used in this research is n-type grown epitaxially on a GaAs substrate.
The purpose of this investigation is to study the electrical properties of GaAs$_{1-x}$P$_x$ alloys and in particular to study magnetoresistance and Hall coefficient and their dependence on the alloy composition and conduction band minima.
CHAPTER I

PROPERTIES OF GaAs\textsubscript{1-x}P\textsubscript{x}

1.1 Crystal Structure

GaAs\textsubscript{1-x}P\textsubscript{x} is a mixed crystal between the III-V compounds GaAs and GaP. Each of these compounds crystallize in the zinc blende structure. Their solid solution GaAs\textsubscript{1-x}P\textsubscript{x} also possesses the zinc-blende structure in which all sites of one face-centered cubic sublattice are occupied by Ga atoms and all sites of the other f.c.c. sublattices are occupied by As or P atoms. In 1955, Folberth demonstrated the existence of the complete mixed crystal system\textsuperscript{1}.

1.2 Lattice Parameter

The lattice parameter is related linearly to the composition factor x. This fact, called Vegard’s rule, was experimentally verified\textsuperscript{2} for GaAs\textsubscript{1-x}P\textsubscript{x}, and is being used as a way to determine the composition factor x. At 25°C the lattice parameter\textsuperscript{2,3} of GaAs is 5.6532 Å and that of GaP is 5.4508 Å. In the temperature range 10-60°C, the lattice parameter of GaP increases linearly\textsuperscript{2} from 5.4504 Å to 5.4517 Å.

1.3 Thermal Data

Information on the thermal properties of the III-V compounds and their alloys is inadequate. The data from thermal expansion measurements\textsuperscript{4} for GaAs are shown in Figure (1-1). The results for Ge are
also included for comparison. The results of Debye temperature measurements for GaAs are shown in Figure 1-2. At 0°C, the Debye temperature $\theta_D(0)$ is equal to 344°C for GaAs, and it is equal to 446°C for GaP.

1.4 Dielectric Constant

At low frequencies the dielectric constant, $K_d(0)$, includes the effect of electronic and ionic polarization. At high frequencies $K_d(\infty)$ includes mainly the effect of electronic polarization. The following values were determined:

For GaAs: $K_d(0) = 12.53$

$K_d(\infty) = 10.90$

For GaP: $K_d(0) = 10.182$

$K_d(\infty) = 8.457$

For GaAs$_{1-x}$P$_x$, the high frequency dielectric constant was found to vary linearly with $x$ at 300°C and at 87°C. And since the ionic contribution to the dielectric constant is almost the same for GaAs and GaP and is much less than the electronic contribution, it is possible to assume that the low frequency dielectric constants for GaAs$_{1-x}$P$_x$ vary linearly from a value of 12.53 for GaAs at $x = 0$ to a value of 10.18 for GaP at $x = 1$. 
Figure (1-1). Temperature dependence of linear expansion coefficient for GaAs and Ge.

Figure (1-2). Temperature dependence of Debye Characteristic Temperature.
CHAPTER II

ENERGY BAND STRUCTURE OF GaAs$_{1-x}$P$_x$

In this chapter the general features of the energy band structure of the GaAs$_{1-x}$P$_x$ system will be discussed and the experimental information available about the forbidden energy gap and the effective masses and their dependence on the composition will be presented.

2.1 First Brillouin Zone

In the perfect GaAs$_{1-x}$P$_x$ crystal, the Ga atoms occupy one face centered cubic sublattice and the other f.c.c. sublattice has a fraction $x$ of its sites being occupied by phosphorus atoms and the rest of its sites being occupied by arsenic atoms.

Both GaAs and GaP have a zinc blende crystal lattice which is a f.c.c. lattice with a basis of two different atoms, one at $(0, 0, 0)$ and the other at $(\frac{a}{4}, \frac{a}{4}, \frac{a}{4})$. The zinc blende lattice has the $\bar{4}3m$ point group symmetry which differs from the $m3m$ of the diamond lattice due to the lack of inversion operation about a point midway between the two basis atoms.

Also GaAs$_{1-x}$P$_x$ has the $\bar{4}3m$ point group symmetry in the sense that when operating any element of this group on this crystal we get the same crystal again with the same properties and the same composition.

The unit cell for GaAs or GaP is the same as that of the face centered lattice. Hence, the Brillouin Zone for GaAs or GaP is
the truncated octahedron shown in Figure (2-1). The commonly used representations for symmetry points and lines are shown.

While the As and P atoms in a GaAs\(_{1-x}P_x\) crystal are distributed randomly over a f.c.c. lattice, which invalidates the usual considerations of band theory, we can still postulate a Brillouin Zone and a band structure for this mixed crystal system on the basis of the experimentally observed sharp band structure. Hence, GaAs\(_{1-x}P_x\) will be assumed to have the same Brillouin Zone as its two end compounds.

2.2 GaAs\(_{1-x}P_x\) Conduction Band

Schematic diagrams of \(E(K)\) curves in the <111> and <100> directions are given in Figure (2-2) for GaAs and in Figure (2-3) for GaP. These diagrams are based on the experimentally determined energy differences between band extrema.

In both cases, the sharp conduction band minimum at \(K = 0\) has a low effective mass. This subband is parabolic near its minimum. But with increasing \(K\) the curvature decreases and the effective mass of the electrons therefore increases. This nonparabolicity is characteristic of most III-V compounds.

GaAs\(_{1-x}P_x\) will be assumed to have a continuous change in \(E(K)\) curves from those of GaAs at \(x = 0\) to those of GaP at \(x = 1\).

2.3 GaAs\(_{1-x}P_x\) Valence Band

In group IV and in III-V semiconductors, the valence band qualitatively has the same structure. Strictly speaking, the valence
Figure (2-1). First Brillouin Zone for Zinc Blende Structure Crystals.
Figure (2-2). Schematic Diagram for the Energy Band Structure of GaAs. 6,8,9,10,11
Figure (2-3). Schematic Diagram for the Energy Band Structure of GaP.6,8,9,10,11
band of the III-V compounds is expected from theory to have eight maxima located on the \textlangle 111 \textrangle axes in the K-space. Each of these eight maxima in InSb is believed to occur at a point 3 \% of the way from K = 0 to the zone boundary along each \textlangle 111 \textrangle direction and these maxima are estimated to be about 10^{-3} \text{eV} higher in energy than the K = 0 point. Because of the closeness of these maxima in both energy and location to the K = 0 point, it is practically possible to assume that the valence band in InSb or in any other III-V compound is qualitatively like that in Si or Ge specially at temperatures much above 0\,^\circ K for which the thermal energy obscures any such fine details of the energy band structure\textsuperscript{8}.

The valence band in these semiconductors consists of two subbands V\textsubscript{1}, V\textsubscript{2} which are degenerate at K = 0 and another spin-orbit-split band V\textsubscript{3} of maximum also at K = 0 but lower than V\textsubscript{1} and V\textsubscript{2}.

Corresponding to the subbands V\textsubscript{1} and V\textsubscript{2}, two kinds of holes are observed experimentally; called heavy and light holes, respectively.

The spin-orbit-split energy in Ga\textsubscript{As\textsubscript{1-x}P\textsubscript{x}} was found to be linearly dependent on the composition\textsuperscript{9,12} from 0.33 \text{eV} for Ga\textsubscript{As} to 0.10 \text{eV} for GaP.

2.4 Ga\textsubscript{As\textsubscript{1-x}P\textsubscript{x}} Energy Gap

Considerable interest lies in the variability of the energy gap of this alloy with composition. The energy gap increases with increasing phosphorus content. At room temperature, Ga\textsubscript{As} has a direct
band gap of $E_g = 1.430$ eV while GaP has an indirect band gap of $E_g = 2.24$ eV.

The dependence of the energy gap $E_g$ on the composition $x$ has been investigated intensively\textsuperscript{8,13,14}. The variation of conduction band edges in GaAs$_{1-x}$P$_x$ with composition is shown in Figure (2-4) as deduced from many different experiments. In this figure the energy is referred to the valence band edge and the energy gap is given by the direct edge line up to $x_0$ and by the [100] edge line from $x_0$ to $x = 1$, where $x_0$ is the composition factor at which the (000) and <100> conduction band minima are at the same energy level. The value of $x_0$ is slightly dependent on the temperature. For room temperature, $x_0$ is approximately 0.44.

Investigations of the absorption spectrum provide a direct method for the determination of the forbidden band. The width of the direct band gap at the centre of the Brillouin Zone $E_1$, between the conduction band minimum and the upper valence band, was determined by this method\textsuperscript{9} for GaAs$_{1-x}$P$_x$. The results show a slight deviation from linearity. The dependence of $E_1$ on the composition $x$ can be described by the empirical expressions:

\begin{equation}
E_1 = (1.51 + 1.16 x + 0.2 x^2) \text{ eV at } 77^\circ K, \quad (2-1)
\end{equation}

and

\begin{equation}
E_1 = (1.43 + 1.15 x + 0.2 x^2) \text{ eV at } 295^\circ K, \quad (2-2)
\end{equation}

where $0 \leq x \leq 1$. 
This is the width of the direct band gap which is the width of the forbidden energy gap \( E_g \) for compositions of \( x < x_o \). But for \( x > x_o \), the forbidden energy is the indirect band gap between the conduction band minima along \(<100>\) and the upper valence band.

The different slopes of the forbidden energy gap \( E_g \) versus composition curve for \( x < x_o \) and \( x > x_o \) could be explained by the fact that the conduction band minima at \((000)\) and along \(<100>\) move up different rates as \( x \) increases.

The temperature dependence of the energy gap \( E_g \) in GaAs and GaP was studied by absorption measurements\(^{15,16,17} \). The usual practice of expressing the temperature dependence of \( E_g \) by a linear variation was found to be inadequate over an extensive temperature range from 0°K to 300°K or higher.

The energy gap temperature dependence was found experimentally\(^{17} \) to have the form

\[
E_g(T) = E_g(0) - \frac{aT^2}{T + \beta} \quad (2-3)
\]

For GaAs the direct energy gap was found to be

\[
E_g(T) = 1.522 - \frac{5.8 \times 10^{-4} T^2}{T + 300}, \quad (2-4)
\]

while for GaP, the indirect energy gap was found to be

\[
E_g(T) = 2.338 - \frac{6.2 \times 10^{-4} T^2}{T + 460} \quad (2-5)
\]

Both expressions fit the experimental results from 0°K to about 900°K.
Figure (2-4). Variation of conduction band edges in GaAs, P$_x$ with composition $x$ as deduced from many different experiments. The solid lines represent the dependence at ~4°K and the dashed lines are for 300°K.
2.5 GaAs$_{1-x}$P$_x$ Effective Masses

For GaAs, early cyclotron resonance and Faraday rotation measurements yielded a best value for the effective mass at the conduction band $\Gamma$ minimum of $0.072 \, m_0$ at 77°K. Recently, the value of the effective mass at this minimum was found to be $(0.066 \pm 0.002) \, m_0$.

The nonparabolic nature of the $\Gamma$ conduction band in GaAs causes the observed mass to be slightly higher than the mass at its centre. The value of this effective mass will be considered $0.072 \, m_0$ to include this nonparabolicity effect.

For GaP, the effective mass values have been determined for the conduction band minima. At the $X$ conduction band the effective mass was found to be $0.35 \, m_0$; and at the $\Gamma$ conduction band it was found to be $0.12 \, m_0$.

The density of states effective mass $m_d$ for a conduction band consisting of $D$ ellipsoidal minima is related to the principal effective masses $m_1, m_2, m_3$ of each ellipsoid by

$$m_d = \left( \frac{D^2 m_1 m_2 m_3}{m_1 m_2 m_3} \right)^{1/3} \tag{2-6}$$

This follows from the fact that the total carrier concentration, $n$, in such a case is obtained by summing over the minima, namely

$$n = \sum_{i=1}^{D} n_i = D n_i,$$

as will be shown later by Equations (4-70) - (4-74) of Chapter IV.

A value of $m_d = 1.2 \, m_0$ is usually accepted for the $X$ conduction band of GaAs. A value of $m_d = 1.4 \, m_0$ has been recently
used for the analysis of measurements made on samples of GaAs$_{0.2}$P$_{0.8}$ doped with selenium. In view of this information, the density of states effective mass $m_d$ at the X conduction band minima for GaAs$_{1-x}$P$_x$ will be assumed independent of $x$ and equal to 1.2 $m_0$.

The effective mass at the $\Gamma$ conduction band, however, was shown\textsuperscript{21} to vary almost linearly with the composition as

$$m^*_\Gamma = 0.072 (1 + x) m_0 .$$

(2-7)

There is no experimental information available about the effective masses for holes in GaAs$_{1-x}$P$_x$, but generally these effective masses can be expected to differ only slightly from the GaAs values\textsuperscript{8} of

$$m^*_v = 0.68 m_0$$

$$m^*_v = 0.12 m_0$$

$$m^*_v = 0.20 m_0 ,$$

because the valence bands have qualitatively the same shape for GaAs and GaP.

2.6 The Energy Difference Between the Conduction Band Minima

The energy separation $\Delta E$ between the conduction $\Gamma$ and X minima can be estimated by

$$\Delta E = E_2 - E_1$$

(2-8)

where $E_1$ and $E_2$ are the energies of the conduction band at $\Gamma$ and X
minima respectively. The variation of \( E_1 \) with the composition is shown by Equations (2-1) and (2-2) for the temperatures 77\(^\circ\)K and 295\(^\circ\)K respectively. The variation of \( E_2 \) with the composition, however, could be expected to be linear as shown in Figure (2-4), namely

\[
E_2 = 1.88 + (2.33 - 1.88) x \quad \text{at} \ 4\(^\circ\)K \quad (2-9)
\]

and

\[
E_2 = 1.78 + (2.24 - 1.78) x \quad \text{at} \ 300\(^\circ\)K \quad (2-10)
\]

Assuming that Equation (2-9) is also the same for 77\(^\circ\)K, then by using Equations (2-1), (2-8) and (2-9) the energy separation \( \Delta E \) at 77\(^\circ\)K could be estimated as

\[
\Delta E = 0.37 - 0.71 x - 0.2 x^2 \quad (2-11)
\]

Similarly at room temperature 297\(^\circ\)K, the energy separation could be estimated from Equations (2-2), (2-8), and (2-10) as

\[
\Delta E = 0.35 - 0.69 x - 0.2 x^2 \quad (2-12)
\]

Equations (2-11) and (2-12) show that \( \Delta E \) does not vary linearly with the composition as it is usually assumed\(^{10,22}\).
CHAPTER III

IMPURITY LEVELS AND BANDS
IN GaAs$_{1-x}$P$_x$

3.1 Ionization Energy

Group VI atoms Te, Se, and S substitute for the As or P and form a solid solution with GaAs$_{1-x}$P$_x$. If these impurities are of low concentration, they form shallow donor levels of ground ionization energy

$$E_d = \frac{m_e^*}{m_n} \frac{e^4}{2\hbar^2 K_d^2} = \frac{m_e^4}{2\hbar^2} \frac{m_e^*}{m_n} \frac{1}{K_d^2}$$

$$= 13.6 \frac{m_e^*}{m_n} \text{ eV} \quad (3-1)$$

This level lies at $-E_d$ from the conduction band edge.

The dielectric constant $K_d$ is 12.5 for GaAs and it is 10.2 for GaP$^{6,23}$. For GaAs$_{1-x}$P$_x$, $K_d$ changes linearly with $x$ as shown in Section 1.4.

The orbital radius for an electron in this ground state is

$$r = \frac{\hbar^2 K_d}{m_e^* e^2} = \frac{\hbar^2}{m_e^*} \frac{m_e}{m_n} K_d$$

$$= 0.528 \frac{K_d}{(m_e^*/m_o)} \text{ Å} \quad (3-3)$$

For GaAs, $\frac{m_e^*}{m_o} = 0.072$

$$E_d = \frac{13.6}{156} 0.072 = 0.0063 \text{ eV}$$

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and
\[ r = 0.528 \frac{12.5}{0.072} = 92 \text{ Å} \]

For GaP, \( \frac{m^*}{m_0} = 0.35 \)

\[ E_d = \frac{13.6}{100} \times 0.35 = 0.05 \text{ eV} \]

and
\[ r = 0.528 \frac{10}{0.35} = 15 \text{ Å} \]

Comparing these orbital radii to the lattice parameters, which are 5.6532 Å for GaAs and 5.4508 Å for GaP and vary linearly in between, we find that while it would be justified to regard the donor electrons in GaAs as being immersed in a uniform medium of dielectric constant \( k \), yet in GaP the orbit of the donor electron encloses a much smaller number of unit cells and the deviations from this hydrogen-like approach could be pronounced.

The ionization energy of Se and Te in GaP have been deduced from Hall effect measurements to be 0.09 eV and 0.08 eV, respectively\(^{20,24}\).

For GaAs, the ionization energy\(^{25}\) of Se and Te was found experimentally to be about 0.004 eV which justifies using the hydrogen like model for such shallow levels.

In GaAs\(_{1-x}\)P\(_x\) the ionization energy \( E_d \) will change as the composition is varied due to the variation of the dielectric constant and the electron effective mass.
3.2 Impurity Bands

If the impurity concentration is large enough such that the electron wave functions of the neighboring impurity centers overlap, the impurity level in the forbidden energy gap broadens to form an impurity band. The ionization energy $E_d$ in this case decreases with increasing donor concentration.

Such impurity banding was observed experimentally for Si and Ge for which $E_d$ vanish at a donor concentration of $7 \times 10^{18}$ cm$^{-3}$ and $6 \times 10^{16}$ cm$^{-3}$ respectively. The difference in these concentrations is because the Bohr radius of electrons at impurity centers in Si is approximately one third that in Ge. Consequently a greater impurity concentration is required in Si for the same wave overlap as in Ge.$^{25}$

Similarly, one can expect that, in $\text{GaAs}_{1-x}\text{P}_x$, $E_d$ will vanish at different donor concentrations as $x$ varies from 0 to 1 since in this case the orbital radius of a ground state electron varies from 92 Å for GaAs to 15 Å for GaP. It has been shown experimentally$^{20,24}$ that $E_d$ decreases with increasing Se and Te impurity concentration in $\text{GaAs}_{0.2}\text{P}_{0.8}$ and $\text{GaAs}_{0.25}\text{P}_{0.75}$, respectively.

3.3 Impurity Bands in the Direct-Indirect Transition

It is interesting to study the impurity levels or bands when the conduction band structure changes from the direct to the indirect gap. Bate$^{26}$ suggested that in III-V compounds with more than one conduction subband of different effective masses one must consider the degeneracy of the different impurity levels (or bands) and the lower conduction subband.
Bate explained this idea for the GaSb in which the conduction band has a (000) minimum of effective mass 0.042 \( m_0 \) and 4 <111> minima, at the Brillouin Zone boundary L points, of effective mass 0.9 \( m_0 \) and of energy higher than the (000) minimum by 0.074 eV. Because of the different effective masses associated with each type of minimum, a free electron in the vicinity of an impurity atom can energetically lie in the impurity band associated with the (000) minimum or in the discrete energy level below the <111> minima. Because of the small effective mass of the (000) minimum, the impurity levels broaden into an impurity band and overlap into this minimum. And because of the high effective mass of the <111> minima, the impurity ground states form a single energy level below these minima which might turn into an impurity band if the donor concentration increases. Electrons in these states can then pass to the (000) conduction band at constant energy. But an electron passing from the (000) impurity band to the (000) conduction band will contribute to the electrical conduction and will leave the impurity atom ionized. While an electron passing from the (000) conduction band to the (000) impurity band or to the <111> impurity levels will not contribute to the conduction and will neutralize the impurity ion. At low impurity concentrations these impurity levels are empty and the mobility is limited by ionized impurity scattering. At high impurity concentration when the impurity bands overlap with the conduction band, a large number of the impurity atoms become neutral and the mobility becomes limited by neutral impurity scattering.
These same considerations could apply to the GaAs$_{1-x}$P$_x$ of x close to $x_c = 0.44$ where the conduction minima have a sufficiently small energy separation. At low impurity concentration, the (000) impurity levels are discrete and lie below the (000) minimum which has an effective mass of

$$m^* = 0.072 (1 + 0.44) m_0$$

$$\sim 0.10 m_0$$

so these levels will have ionization energy of

$$E_{d1} = \frac{13.6}{k^2} \frac{m^*}{m_0}$$

$$= \frac{13.6}{(11.6)^2} (0.1) = 0.010 \text{ eV}$$

and an orbital radius of

$$r_1 = 0.528 \frac{11.6}{0.1} = 61 \text{ Å},$$

assuming the dielectric constant to vary linearly between 12.5 for GaAs and 10 for GaP.

The <100> impurity levels will have an ionization energy of

$$E_{d2} = \frac{13.6}{(11.6)^2} 0.35 = 0.035 \text{ eV}$$

and an orbital radius of

$$r_2 = 0.528 \frac{11.6}{0.35} = 17.5 \text{ Å}$$

At high impurity concentration, the ionization energy looses its meaning since the electrons can pass between an impurity band and a conduction band without changing their energy and a large number of these impurity atoms becomes neutral.
a) Energy Band of GaAs$_{1-x}$P$_x$ for $x < x_0$

b) Energy bands of GaAs$_{1-x}$P$_x$ for $x > x_0$

Figure (3.1). Energy Band Configuration for GaAs$_{1-x}$P$_x$ for $x < x_0$ and for $x > x_0$. 
3.4 Electron Density in N-Type GaAs$_{1-x}$P$_x$ at Different Temperatures.

An n-type semiconductor will usually contain more than one donor species. Also it will always contain acceptor impurities of various kinds. Some impurities may be able to provide or accept more than one electron. Moreover electrons can be trapped by an impurity not only in ground states but also in excited states. Also these states could be influenced by the existence of more than one minima in the conduction band like the case of silicon containing partly compensated phosphorus donors, where the ground state was shown to split into two states of 0.010 eV energy separation.\(^1\)

A simple analysis to determine the electron densities and energies in n-type GaAs$_{1-x}$P$_x$ will be carried out here. But, it must be remembered that this is by no means a simple matter and a great deal of information about this semiconductor is needed to decide whether a simple analysis is appropriate.

Consider n-type GaAs$_{1-x}$P$_x$ of principal donor levels at an energy $E_d$ below the lower conduction band edge. The Fermi level $\xi$ will be assumed to lie well above the energies of all other kinds of impurity states at all temperatures of the extrinsic range. In this case all donors among these states will retain their electrons and be electrically neutral, and all the acceptor impurities will acquire extra electrons as consistent with their energy states below the Fermi level. Let the density of electrons required to satisfy these acceptors be $N_a$. In the extrinsic range, these $N_a$ electrons have to come from the principal donors of density $N_d$. 
The remaining electrons \((N_d - N_a)\) will be distributed between the donor levels at \((E_C - E_d)\) and the conduction band valleys at (000) and along <100>.

Let the density of electrons in the (000) valley be \(n_1\) and let their density in the <100> valleys be \(n_2\). The energy separation \(\Delta E\) between the two sets of valleys is a function of the composition \(x\) as discussed before. Also \(\Delta E\) varies slightly with the temperature over the extrinsic range.

Consider the valence band edge at (000) to be the reference of energy.

The ionized donors concentration \(N_{di}\) is related to the number of donor atoms concentration \(N_d\) by 25,27

\[
N_{di} = \frac{N_d}{1 + 2 e^{\left(\frac{\xi - (E_C - E_d)}{kT}\right)}}
\]

(3-5)

\[
= \frac{N_d}{1 + 2 e^{\eta + \varepsilon_d}}
\]

(3-6)

where

\[
\varepsilon_d = \frac{E_d}{kT}
\]

(3-7)

and

\[
\eta = \frac{\xi - E_C}{kT}
\]

(3-8)

and \(E_C\) is the conduction band edge \(E_1\) or \(E_2\) whichever is lower.

In the extrinsic range, the neutrality condition requires that the number of ionized donors be equal to the number of electrons in the conduction valleys \(n_1, n_2\) plus the electrons taken by the acceptors \(N_a\).
Then
\[ n_1 + n_2 + N_a = \frac{N_d}{1 + 2 e^{(\eta + \epsilon_d)/e}} \quad (3-9) \]

\[ n_1 = \frac{1}{2\pi^2} \left( \frac{2m_1 kT}{\hbar^2} \right)^{3/2} \int_{E_1}^{\infty} (E - E_1)^{1/2} f_o(E) dE \quad (3-10) \]

\[ n_2 = \frac{1}{2\pi^2} \left( \frac{2m_2 kT}{\hbar^2} \right)^{3/2} \int_{E_2}^{\infty} (E - E_2)^{1/2} f_o(E) dE \quad (3-11) \]

where \( m_1 \) and \( m_2 \) are the density-of-states effective masses of the corresponding conduction band edges.

Let \( \eta_1 = \frac{\xi - E_1}{kT} \) and \( \eta_2 = \frac{\xi - E_2}{kT} \quad (3-12) \)

then

\[ \eta_1 - \eta_2 = \frac{E_2 - E_1}{kT} = \frac{\Delta E}{kT} \equiv S = S(x) \quad (3-13) \]

where \( S \) is the reduced energy separation between conduction band edges.

Let \( a_1 = \frac{m_1}{m_o} \) and \( a_2 = \frac{m_2}{m_o} \quad (3-14) \)

and

\[ G = \frac{1}{2\pi^2} \left( \frac{2\text{K}T}{\hbar^2} \right)^{3/2} \quad (3-15) \]

where \( m_o \) = free electron mass.

From the equations (10)-(15) the conduction band electrons are
\[ n_1 = \frac{3/2}{\pi} G(\alpha_1 T) \left( \frac{1 - \frac{1}{4} \pi^2}{\frac{1}{2}} \right) \]  
(3-16)

\[ n_2 = \frac{3/2}{\pi} G(\alpha_2 T) \left( \frac{1 - \frac{1}{4} \pi^2}{\frac{1}{2}} \right) \]  
(3-17)

The reduced energies \( n_1 \) and \( n_2 \) are the reduced energy separation between the conduction band edges and the Fermi level.

The Fermi integrals \( F_k(\eta) \) are defined by

\[ F_k(\eta) = \int_0^\infty \frac{x^k \, dx}{1 + e^{x - \eta}} \]  
(3-18)

Values of this integral are tabulated in many references 25, 27, 28.

In principle, Equation (3-9) could be solved to obtain \( \eta \) and hence the Fermi level. But with the Fermi integrals as defined it is difficult to solve this equation and approximate formulas for the Fermi integrals must use

For \( \eta \leq -3.5 \), \( F_{1/2}(\eta) \) could be replaced by

\[ F_{1/2}(\eta) = \frac{\sqrt{\pi}}{2} e^{\eta} \]  
(3-19)

with an error less than 1%. As \( \eta \) goes more negative the error decreases.

Still better approximation for \( F_{1/2}(\eta) \) is

\[ F_{1/2}(\eta) = \frac{\sqrt{\pi}}{2} e^{\eta} = \frac{\sqrt{\pi}}{2} \, \frac{1}{1 + C e^{\eta}} \]  
(3-20)

with differing values of \( C \) to optimize the fit for various ranges of \( \eta \). For the whole range from classical conditions up to \( \eta \leq +1.3 \), the best compromise is effected with the value \( C = 0.27 \) giving an error of \( \pm 3\% \).
With the magnitude \( \frac{\Delta E}{kT} = |S| \geq 3 \), it is possible to use (3-19) and (3-20) to get the approximation:

\[
F_{1/2}(n - |S|) = e^{-1} F_{1/2}(\eta) = \frac{\sqrt{\pi}}{2} \frac{e^{-|S|}}{C + e^{-\eta}}
\]

valid for \( n \leq +1.3 \), with an error within \( \pm 3\% \).

In the range \( n \leq -2.5 \), it is easier to use the approximation (3-19) together with

\[
F_{1/2}(n - |S|) = F_{1/2}(\eta) = \frac{\sqrt{\pi}}{2} e^{-|S|}
\]

valid for any value of \( |S| \) and the error lies within \( \pm 3\% \) for \( n \leq -2.5 \).

The neutrality condition (9) could generally be written

\[
\left( a_{1T} \right)^{3/2} GF_{1/2}(\eta_1) + \left( a_{2T} \right)^{3/2} GF_{1/2}(\eta_2) + N_a = \frac{Nd}{1 + 2e^{(n+\epsilon_d)}}
\]

where \( n = \eta_1 \) if \( E_1 < E_2 \)

and \( n = \eta_2 \) if \( E_1 > E_2 \)

If the conditions of approximation (3-21) are satisfied, the neutrality condition (3-23) will be

\[
\left( a_{1T} \right)^{3/2} \frac{\sqrt{\pi}}{2} \frac{G}{C + e^{-\eta_1}} + \left( a_{2T} \right)^{3/2} \frac{\sqrt{\pi}}{2} \frac{Ge^{\eta_1}}{C + e^{-\eta_1}} + N_a = \frac{Nd}{1 + 2e^{(n_1+\epsilon_d)}}
\]

which is written for the case \( E_1 < E_2 \), and could be rewritten as

\[
\frac{A_{12}}{C + e^{-\eta_1}} + N_a = \frac{Nd}{1 + 2e^{(n_1+\epsilon_d)}}
\]
where

\[ A_{12} = [(\alpha_1 T)^{3/2} + (\alpha_2 T)^{3/2} - |S| \frac{\sqrt{\pi}}{2} G \]

From Equation (3-25), the value of \( e^{-\eta_1} \) is

\[ e^{-\eta_1} = \frac{1}{2(N_d-N_a)} \left\{ [A_{12} - C(N_d-N_a) + 2N_a e^{\varepsilon_d}] + [(A_{12} - C(N_d-N_a) + 2N_a e^{\varepsilon_d})^2 \right. \]

\[ + 8(A_{12} + CN_a) (N_d-N_a) e^{\varepsilon_d}]^{1/2} \}

and the electron density \( n_1 \) will be

\[ n_1 = \frac{\sqrt{\pi} (\alpha_1 T)^{3/2} G}{C + e^{-\eta_1}} \]

\[ = \frac{\sqrt{\pi} G (\alpha_1 T)^{3/2}}{C + e^{-\eta_1}} \]

\[ \left\{ A_{12} + C(N_d-N_a) + 2N_a e^{\varepsilon_d} + [(A_{12} - C(N_d-N_a) + 2N_a e^{\varepsilon_d})^2 + 8(A_{12} + CN_a) (N_d-N_a) e^{\varepsilon_d}]^{1/2} \right\} \]

and

\[ n_2 = (\frac{\alpha_2}{\alpha_1})^{3/2} - |S| e^{\eta_1} \]

and

\[ n = n_1 + n_2 = n_1 \left[ 1 + (\frac{\alpha_2}{\alpha_1})^{3/2} - |S| e^{\eta_1} \right] \]

For the other case when \( E_1 < E_2 \), the Equations (3-24) to (3-31) apply provided the subscripts 1 and 2 are interchanged in the \( \alpha \)'s and the \( n \)'s and \( A_{21} \) is used instead of \( A_{12} \).
If the condition of approximation (3-22) is satisfied, i.e., \( \frac{c-E}{kT} = \eta_c \leq -2.5 \), the neutrality Equation (3-23) will be

\[
\begin{align*}
&\left(\alpha_1 T\right) \frac{3}{2} \sqrt{\frac{\pi}{2}} e^{\eta_1} + \left(\alpha_2 T\right) \frac{3}{2} \sqrt{\frac{\pi}{2}} e^{-|S|} + \eta \\eta_a \\
&= \frac{N_a}{1 + 2e^{\eta_1 + \eta_d}} \\
\end{align*}
\]

(3-32)

then

\[
\begin{align*}
A_{12} e^{\eta_1} + \eta_a &= \frac{N_a}{1 + 2e^{\eta_1 + \eta_d}} \\
(3-33)
\end{align*}
\]

\[
e^{\eta_1} = \frac{2(N_d-N_a)}{A_{12}} \left[ 1 + \frac{2N_a e^{\eta_d}}{A_{12}} \right] \left[ 1 + \frac{2N_a e^{\eta_d}}{A_{12}} \right]^{1/2} + \frac{8(N_d-N_a) e^{\eta_d}}{A_{12}} \]

(3-34)

so

\[
n_1 = \sqrt{\frac{\pi}{2}} G(\alpha_1 T) e^{\eta_1} \\
(3-35)
\]

and

\[
n_2 = \sqrt{\frac{\pi}{2}} G(\alpha_2 T) e^{-|S|} \\
(3-36)
\]

Also for this case, the Equations (3-32) to (3-36) are written when \( E_1 < E_2 \). For the other case \( E_1 > E_2 \), they still hold provided the subscripts of \( \alpha \)'s and \( \eta \)'s are interchanged and \( A_{21} \) is used instead of \( A_{12} \).
CHAPTER IV
ELECTRICAL TRANSPORT THEORY FOR A CUBIC SEMICONDUCTOR IN SMALL FIELDS

In this chapter the electron transport theory in weak magnetic and electric fields will be presented. The medium will be assumed to be an isothermal semiconductor of the cubic crystal structure and of permeability equal to that of free space. The discussion here will be limited to the assumptions and the results of this theory. Detailed derivations are to be found in many references,29-33

4.1 Conductivity and Resistivity Tensors

Consider an anisotropic solid placed in a magnetic field of density B. The forces acting on the charge carriers will be the electrochemical field \( \mathbf{E} \) and the temperature gradient \( \nabla T \). The electric current density \( \mathbf{J} \) and the heat current density \( \mathbf{q} \) will be related to these forces by the linear equations

\[
J_i = \sigma_{ij}(B) \mathbf{E}_j + M_{ij}(B) \frac{\partial T}{\partial x_j},
\]

and

\[
q_i = N_{ij}(B) \mathbf{E}_j + L_{ij}(B) \frac{\partial T}{\partial x_j},
\]

where a rectangular coordinate system \((x_1, x_2, x_3)\) is assumed, and summation over repeated indices is implied.

The tensor coefficients in these equations simply express the fact that the transport currents are not generally in the same directions as those of the forces.
In this discussion, the case of warm or hot electrons will be excluded. It will be assumed that the average energy of the charge carriers does not exceed the equilibrium energy which is \( \frac{3}{2} kT \) for the nondegenerate case of lattice temperature \( T \).

This discussion is limited to the resistivity, Hall effect and magnetoresistance of a cubic semiconductor placed in a weak magnetic field and in an isothermal condition. For this purpose we only need to discuss the transport equation:

\[
J_i = \sigma_{ij}(B) \xi_j^* .
\] (4-3)

The electrochemical field \( \xi_j^* \) is related to the externally applied electric field \( \xi_j \) and to the chemical potential or Fermi potential \( \zeta \) of the electrons by:

\[
\xi_j^* = \xi_j - \frac{1}{(-e)} \frac{\partial \zeta}{\partial x_j} = \xi_j + \frac{1}{e} \frac{\partial \zeta}{\partial x_j} .
\] (4-4)

where \( e \) is the magnitude of the electronic charge. For homogeneous material, the Fermi level \( \zeta \) is independent of position and thus \( \xi_j^* = \xi_j \) = the externally applied electric field. So the transport equation reduces to:

\[
J_i = \sigma_{ij}(B) \xi_j .
\] (4-5)

In the laboratory, where it is much easier to control the electric current rather than the electric field, most measurements are carried out under the condition that the electric current is the independent variable. In this case, Equation (4-5) could be written as:
\[ \xi_i = \rho_{ij}(B)J_j \quad (4-6) \]

The tensors \( \sigma_{ij}(B) \) and \( \rho_{ij}(B) \) are called the conductivity and the resistivity tensors respectively and, at any magnetic field density \( B \), they are related by

\[ \sigma_{ij}(B)\rho_{jk}(B) = \delta_{ik} \quad (4-7) \]

where \( \delta_{ik} \) is the 3-dimensional unit tensor

\[ \delta_{ik} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} . \]

Onsager's relations yield the following equalities for the conductivity and resistivity tensors

\[ \sigma_{ij}(B) = \sigma_{ji}(-B) \quad (4-8) \]

and

\[ \rho_{ij}(B) = \rho_{ji}(-B) \quad (4-9) \]

Therefore \( \sigma_{ij}(0) \) and \( \rho_{ij}(0) \) are symmetric.

The tensors \( \sigma_{ij}(B) \) and \( \rho_{ij}(B) \) could be expanded as a Taylor series in the components of the magnetic field \( B_1, B_2, B_3 \). For small magnetic fields, terms of \( B^3 \) or higher order will be small compared to terms of zero, first or second order dependence.

Thus, neglecting \( B^3 \) or higher order terms, the conductivity and resistivity tensors for small magnetic field could be written as:

\[ \sigma_{ij}(B) = \sigma_{ij} + \sigma_{ijk}B_k + \sigma_{ijk\ell}B_kB_\ell \quad (4-10) \]
\[ \rho_{ij}(B) = \rho_{ij} + \rho_{ijkl} B_k B_l, \quad (4-11) \]

where \( \sigma_{ij}, \sigma_{ijk}, \sigma_{ijkl} \) are called the conductivity tensor coefficients, given by

\[ \sigma_{ij} = \sigma_{ij}(B) \bigg|_{B = 0} = \sigma_{ij}(0), \quad (4-12) \]

\[ \sigma_{ijk} = \frac{\partial \sigma_{ij}(B)}{\partial B_k} \bigg|_{B = 0}, \quad (4-13) \]

and

\[ \sigma_{ijkl} = \frac{1}{21} \frac{\partial^2 \sigma_{ij}(B)}{\partial B_k \partial B_l} \bigg|_{B = 0} = \sigma_{ijkl}, \quad (4-14) \]

Similar definitions hold for the resistivity tensor coefficients \( \rho_{ij}, \rho_{ijk}, \rho_{ijkl} \).

4.2 Symmetry Considerations

Both GaAs and GaP belong to the zinc blende type of crystal lattice in which all sites of one face-centered cubic sublattice are occupied by Ga atoms and all sites of the other sublattice are occupied by As or P atoms. Away from each Ga atom there is an arsenic or phosphorous atom at a displacement vector of \( \left( \frac{a}{4}, \frac{a}{4}, \frac{a}{4} \right) \) as shown in Figure (4-1), where \( a \) is the unit cell cube side.

GaAs and GaP have the symmetry of the point group \( \overline{4} 3 m \). The generating elements of this group are:
1) 4-fold rotation inversion about x-axis. This could be represented by the matrix:

\[
[a_1] = \begin{bmatrix}
-1 & 0 & 0 \\
0 & 0 & -1 \\
0 & 1 & 0
\end{bmatrix}
\] (4-15)

\[|a_1| = -1\]

2) 3-fold rotation about <111> axis. This element could be represented by the matrix:

\[
[a_2] = \begin{bmatrix}
0 & 1 & 0 \\
0 & 0 & 1 \\
1 & 0 & 0
\end{bmatrix}
\] (4-16)

\[|a_2| = 1\]

3) Reflection in the (110) plane. This could be represented by the matrix:

\[
[a_3] = \begin{bmatrix}
0 & 1 & 0 \\
1 & 0 & 0 \\
0 & 0 & 1
\end{bmatrix}
\] (4-17)

\[|a_3| = -1\]
Figure (4-1). Face centered sublattice of Ga atoms in GaAs$_{1-x}$P$_x$.
Away from each Ga atom there is an As or P atom at a vector displacement of $\left(\frac{a}{4}, \frac{a}{4}, \frac{a}{4}\right)$.
Only one such atom is shown here.
The point group \( T \bar{3} m \) has 24 elements, namely:

- **E** which is the identity element.
- **3C\(_2\)** where \( C\(_2\) \) is a 2-fold rotation around \( x, y, \) or \( z \) axes.
- **8C\(_3\)** where \( C\(_3\) \) is a 3-fold rotation about a \( <111> \) axis.
- **6σ\(_d\)** where \( σ\(_d\) \) represents a reflection in a \( (110) \) plane.
- **6S\(_4\)** where \( S\(_4\) \) represents a 4-fold improper rotation around a \( <100> \) axis.

Any of these elements could have a matrix representation which is one or which could be generated by the matrices \([a_1], [a_2], \) and \([a_3]\).

By definition, if the point group operation represented by its matrix element is performed on the crystal belonging to this point group, the atoms of this crystal will be brought back to their original arrangement and there will be no change in the crystal properties as seen by the laboratory.

\( \text{GaAs}_{1-x} \text{P}_x \) belongs to the group \( T \bar{3} m \) like GaAs and GaP, since performing any element of this point group on \( \text{GaAs}_{1-x} \text{P}_x \) crystal yields the same crystal with the same properties even though a phosphide atom might take the place originally occupied by an arsenic atom or the other way around. Based on this fact, it will be possible to apply the analysis presented here for the case of ordered cubic structures, like the diamond and zinc-blende lattices, on the case of \( \text{GaAs}_{1-x} \text{P}_x \) where the sites of one sublattice could be randomly occupied by an arsenic or phosphorus atom. This is possible provided that the material is macroscopically homogeneous.
The symmetry properties of the conductivity and resistivity tensor coefficients are obtained from performing the elements of this group on the laboratory system i.e. on $\xi, \eta, \zeta$. These symmetry properties are:

\[ \rho_{ij} = \rho_{\delta ij} \quad \text{and} \quad \sigma_{ij} = \sigma_{\delta ij}, \quad (4-18) \]

where

\[ \delta_{ij} = 1 \quad \text{if} \quad i = j \]

\[ \delta_{ij} = 0 \quad \text{if} \quad i \neq j, \]

and

\[ \rho_{ijk} = \rho_{123 \epsilon_{ijk}} \quad \text{and} \quad \sigma_{ijk} = \sigma_{123 \epsilon_{ijk}}, \quad (4-19) \]

where

\[ \epsilon_{ijk} = 1 \quad \text{if} \quad i, j, k \quad \text{form a positive sequence of} \quad 1, 2, 3; \]

\[ \epsilon_{ijk} = -1 \quad \text{if} \quad i, j, k \quad \text{form a negative sequence of} \quad 1, 2, 3; \]

\[ \epsilon_{ij} = \epsilon_{ji} = \epsilon_{jj} = 0, \]

and

\[ \rho_{1111} = \rho_{\epsilon_{iii}} \quad \text{for} \quad i = 1, 2, \text{or} \quad 3; \quad (4-20) \]

\[ \rho_{1122} = \rho_{\epsilon_{iij}} \quad \text{for} \quad i \neq j; \quad (4-21) \]

\[ \rho_{1212} = \rho_{\epsilon_{ijj}} \quad \text{for} \quad i \neq j. \quad (4-22) \]

The coefficients $\rho_{1121}, \rho_{1232}$ or any coefficient $\rho_{ijkl}$ containing 3 equal indices or 3 nonequal indices are zero. Similar relations hold for $\sigma_{ijkl}$.

The relations between the conductivity tensor coefficients and the resistivity tensor coefficients could be derived
by using these symmetry properties together with Equations (4-7), (4-10), and (4-11). These relations are:

\[ \rho_o = \frac{1}{\sigma_o} \quad \text{or} \quad \sigma_o = \frac{1}{\rho_o}, \quad (4-23) \]

\[ \rho_{123} = -\frac{\sigma_{123}}{\sigma_o^2} \quad \text{or} \quad \sigma_{123} = -\frac{\rho_{123}}{\rho_o^2}, \quad (4-24) \]

\[ \rho_{1111} = -\frac{\sigma_{1111}}{\sigma_o^2} \quad \text{or} \quad \sigma_{1111} = -\frac{\rho_{1111}}{\rho_o^2}, \quad (4-25) \]

\[ \rho_{1122} = -\frac{\sigma_{123}}{3} - \frac{\sigma_{1122}}{\sigma_o^2}, \quad (4-26) \]

\[ \sigma_{1122} = -\frac{\rho_{123}}{3} - \frac{\rho_{1122}}{\rho_o^2}, \quad (4-27) \]

and

\[ \rho_{1212} = \frac{\sigma_{123}}{2\sigma_o^3} - \frac{\sigma_{1212}}{\sigma_o^2}, \quad (4-28) \]

\[ \sigma_{1212} = \frac{\rho_{123}}{3} - \frac{\rho_{1212}}{\rho_o^2}. \quad (4-29) \]

4.3 Hall Effect and Magnetoresistance

The relation \( \xi_{ij} = \rho_{ij} (B) J_i \) for a cubic semiconductor in a small magnetic field could now be written as
\[ \xi_i = (\rho_{ij} + \rho_{ijk}B_k + \rho_{ijk}B_kB_k) J_j \]

\[ = (\rho_0\delta_{ij} + \rho_{123} \epsilon_{ijk}B_k + \rho_{ijk}B_kB_k) J_j \]

then

\[ \xi_i = \rho_0 J_i + \rho_{123} \epsilon_{ijk}J_jB_k + \rho_{ijk}J_kB_kB_k \] (4-30)

\[ \rho_0 J_i \] is the component of the electric field due to the zero magnetic field resistivity \( \rho_0 \).

\[ \rho_{123} \epsilon_{ijk}J_jB_k \] or \( \rho_{123} - \frac{J \times B}{B} \) is the component of the electric field due to Hall effect. The Hall coefficient \( R(B) \) is usually defined by,

\[ \xi_H = R(B) \frac{B \times J}{J} = \text{Hall electric field} \] (4-31)

For small fields, \( R(B) = R(B) \bigg|_{B=0} = R_0 = -\rho_{123} \).

\[ \rho_{ijk}J_jB_kB_k \] is the component of the electric field due to the magnetoresistivity i.e., due to the change in the resistance when applying magnetic field \( B \).

In the laboratory, the resistivity \( \rho(B) \) along certain directions is defined as the ratio of the electric field to the current density along that direction. The component of the electric field in the direction of the current density \( J \) is \( \frac{\xi \cdot J}{J} \) or \( \frac{\xi_i J_i}{J} \). Then, resistivity along current direction is

\[ \rho(B) = \frac{\xi \cdot J}{J^2} = \frac{\xi_i J_i}{J^2} \] (4-32)

\[ = \rho_0 + \rho_{ijk} \frac{J_i J_i}{J^2} B_kB_k \] (4-33)
where the identity $[\varepsilon_{ijk}J_{i}J_{k} = 0]$ was used.

The change in resistivity along a current direction, due to the application of a magnetic field of density $B$, could be written as

$$\Delta \rho = \rho(B) - \rho_o = \rho_{ijkl} \frac{J_i J_j}{J^2} B_k B_l .$$

(4-34)

By writing the summation over repeated indices explicitly, then

$$\frac{\Delta \rho}{\rho_o B^2} = \frac{\rho(B) - \rho_o}{\rho_o B^2} = \sum_{i,j,k,l} \frac{\rho_{ijkl} J_i J_j B_k B_l}{\rho_o J^2 B^2} .$$

(4-35)

If the components of $J$, $B$ are referred to the cubic crystallographic axes, then it is possible to make use of the fact that there are only 3 independent components of $\rho_{ijkl}$, namely:

$\rho'_{1111}, \rho'_{1122}, \rho'_{1212}$

to simplify the expression of $\frac{\Delta \rho}{\rho_o B^2}$ with the help of Equations (4-20), (4-21), and (4-22). Then

$$\frac{\Delta \rho}{\rho_o B^2} = \frac{\rho(B) - \rho_o}{\rho_o B^2} = \frac{\rho_{1122}}{\rho_o} + \frac{2\rho_{1212}}{\rho_o} \left( \sum_{i} \xi_i \eta_i \right)^2$$

$$+ \frac{\rho_{1111} - \rho_{1122} - 2\rho_{1212}}{\rho_o} \sum_{i} \xi_i \eta_i \xi_i \eta_i \xi_i \eta_i ,$$

(4-36)

where $(\xi_1, \xi_2, \xi_3)$ are the direction cosines of the current density.
$J$, $n_1$, $n_2$, $n_3$ are the direction cosines of the magnetic field density $B$. Both of these direction cosines are referred to the crystal cubic axes.

Define the coefficients in the right hand side of this equation as:

$$b = \frac{\rho_{1122}}{\rho_0}$$ (4-37)

$$c = \frac{2\rho_{1212}}{\rho_0}$$ (4-38)

$$d = \frac{\rho_{1111} - \rho_{1122} - 2\rho_{1212}}{\rho_0}$$ (4-39)

These are called Seitz magnetoresistance coefficients. Equation (4-36) reduces to

$$\frac{\Delta \rho}{\rho_0 B^2} = b + c \left( \sum_i \xi_i n_i \right)^2 + d \sum_i \xi_i^2 n_i^2 .$$ (4-40)

The coefficients $b$, $c$, and $d$ could be measured in the laboratory, from which the coefficients $\rho_{ijkl}$ or $\sigma_{ijkl}$ could be determined. In the next section the method of the Boltzmann Transport Equation will be introduced. With the assumption of a relaxation time, this method will be used to express the conductivity and resistivity tensor coefficients in terms of the electronic properties of the material.
4.4 The Boltzmann Transport Equation and the Relaxation Time Approximation

The motion of a large number of electrons is described by

\[
\frac{df}{dt} = \left( \frac{\partial f}{\partial t} \right)_{\text{fields}} + \left( \frac{\partial f}{\partial t} \right)_{\text{coll}},
\]

(4-41)

where \( f = f(K, r, t) \) is the electron distribution function. It is the probability that the states at \( (K, r) \) in the phase space are being occupied at the time \( t \). The phase space contains the wave vector space \( K \) and the coordinate space \( r \) together. A vector in the phase space \( (K, r) \) is defined by the 3 components \( K_x, K_y, K_z \) indicating the electron wave number vector and by the 3 components \( x, y, z \) indicating the electron position. The above equation describes the fact that the rate of change of the electron distribution function equals the rate of change due to the action of external forces plus the rate of change due to collision or scattering of the electrons.

The first term in the right hand side of Equation (4-41), describing the effect of the externally applied forces on the electron position and wave vector, is given by

\[
\left( \frac{\partial f}{\partial t} \right)_{\text{fields}} = -K \cdot \nabla_K f - v \cdot \nabla_r f
\]

(4-42)

where \( v \) is the velocity of electron; \( \nabla_K \) and \( \nabla_r \) are gradients in the wave vector and coordinate spaces respectively; \( \dot{K} \) is the time rate of change of electron wave vector. Equation (4-41) could now be written as
This equation is known\(^3\) as Boltzmann's equation and is the fundamental equation governing all transport phenomena.

For small externally applied electric and magnetic fields, the time rate of change of electron wave vector is given by the approximation\(^3\)

\[
\hbar \mathbf{K} = e \mathbf{E} + \mathbf{v} \times \mathbf{B} \quad \text{.} 
\]  

(4-44)

For a homogeneous crystal at constant temperature and placed in an externally applied electric and magnetic fields in a steady state condition, Boltzmann's equation will reduce to

\[
- e \mathbf{E} \cdot \mathbf{v}_f = (\frac{\partial f}{\partial t})_{\text{coll}} \quad \text{.} 
\]  

(4-45)

In the absence of the external forces, the solution of Equation (4-45) is given by the Fermi-Dirac distribution function \(f_0(E)\),

\[
f_0(E) = \frac{1}{1 + e^{\frac{E - \xi}{kT}}} \quad . \]  

(4-46)

For small applied field, the distribution function will be slightly perturbed from \(f_0\) and as a first approximation could be written as

\[
f = f_0 + f_1 \quad \text{where } f_1 \ll f_0 \quad . \]  

(4-47)

The perturbation \(f_1\) will be obtained by solving Boltzmann's Equation
This solution is greatly simplified if the collision term can be expressed in terms of a relaxation time, namely

$$\left(\frac{\partial f}{\partial t}\right)_{\text{coll}} = -\frac{f - f_0}{\tau} = -\frac{f_1}{\tau}, \quad (4-48)$$

where the relaxation time $\tau$ is generally a function of the wave vector $K$.

Under these conditions, Boltzmann's equation (4-45) reduces to

$$-\frac{e}{\hbar} \mathbf{v} \times \mathbf{B} \cdot \nabla f + \xi \cdot \nabla f \frac{\partial f}{\partial E} = -\frac{f_1}{\tau}, \quad (4-49)$$

where the following equations and approximation were used

$$\nabla f = \nabla f_0 + \nabla f_1,$$

$$\nabla f_0 = \frac{\partial f_0}{\partial E}, \quad \nabla f = \frac{\partial f}{\partial E} = [\hbar \mathbf{v}],$$

$$\mathbf{v} \times \mathbf{B} \cdot \mathbf{v} \equiv 0,$$

and

$$-\frac{e}{\hbar} \xi \cdot \nabla f = -\frac{e}{\hbar} \xi \cdot \nabla f_0 = -e \xi \cdot v \frac{\partial f_0}{\partial E}.$$

The solution to Equation (4-49), which is valid for small magnetic fields such that $\frac{eB}{m^*} < 1$, could be written as

$$f_1 = - (e) \xi_1 \frac{\partial f_0}{\partial E} \left[ \tau v_1 - \tau \Omega (\tau v_1) + (\tau \Omega)^2 (\tau v_1) \right]$$

$$- (\tau \Omega)^3 (\tau v_1) + \cdots \right] \quad (4-50),$$

where $\Omega$ is an operator given by
The electric current density is given by

\[
\mathbf{J}_i = -\frac{e}{4\pi^3} \iiint_{\text{Brillouin Zone}} \mathbf{v}_i f \, d^3K = \frac{-e}{4\pi^3} \iiint_{\text{Brillouin Zone}} \mathbf{v}_i f_0 \, d^3K
\]

\[= \sigma_{ij} (B) \epsilon_{ij}, \quad (4-52)\]

where \(d^3K\) represents a differential element of volume in the wave vector space. The equilibrium distribution \(f_0\) gives no contribution to the current because \(\mathbf{v}_i\) is an odd function of \(K\) while \(f_0\) is an even function of \(K\); or physically because the net current in a material is zero if there is no external forces applied.

From Equations (4-50), (4-51), and (4-52); and by comparison to the Taylor expansion of \(\sigma_{ij} (B)\) for small magnetic field which is given by Equation (4-10), it is possible to get expressions for the conductivity tensor coefficients \(\sigma_{ij}, \sigma_{ijk}\) and \(\sigma_{ijk\ell}\) as functions of the relaxation time \(\tau\), equilibrium distribution function \(f_0\) and energy band structure.

In the next section, special configurations of conduction band structures for the cubic semiconductor will be considered and the conductivity and resistivity tensor coefficients for each configuration will be presented.
4.5 Conductivity and Resistivity Tensor Coefficients for Some Special Conduction Band Structures

4.5.1 Spherical Conduction Band

Consider a conduction band of energy \( E \) given by

\[
E = E_c + \frac{\hbar^2 K^2}{2m^*},
\]

(4-53)

where \( \mathbf{K} = (K_x, K_y, K_z) \) is the electron wave vector and \( m^* \) is the electron effective mass.

The electron density \( n \) will be given by

\[
n = \int_{E_C}^{\infty} L_S(E) f_o(E) \, dE,
\]

(4-54)

where \( L_S(E) \), the density of electron states, is given in this case by

\[
L_S(E) = \frac{1}{2\pi^2} \left[ \frac{2m^*}{\hbar^2} \right]^{3/2} (E - E_c)^{1/2} = \Lambda_S (E - E_c)^{1/2}.
\]

(4-55)

So, the electron density is

\[
n = \Lambda_S \int_{E_C}^{\infty} (E - E_c)^{1/2} f_o(E) \, dE,
\]

(4-56)
where \( n \) is the reduced energy separation between the edge of the conduction band \( E_C \) and the Fermi level \( \zeta \). It is given by

\[
\eta = \frac{\zeta - E_C}{kT}.
\]

The Fermi integrals \( F_\alpha (\eta) \) is defined as

\[
F_\alpha (\eta) = \int_0^\infty \frac{x^\alpha}{1 + e^{x-\eta}} \, dx,
\]

where \( x \) is the reduced energy of the charge carrier given by \( \frac{E - E_C}{kT} \). The values of these integrals for many indices \( \alpha \) have been tabulated in many references. For the nondegenerate case, when the Boltzmann distribution \( f_0 (E) = e^{-\frac{E-\zeta}{kT}} \) could be used, \( F_{1/2} (\eta) \) reduces to \( \frac{\sqrt{\pi}}{2} e^{\eta} \).

For the case of a spherical conduction band, the zero magnetic field conductivity is given by

\[
\sigma_{ij} = \frac{ne^2}{m^*} \delta_{ij} = \sigma_\star \delta_{ij},
\]

where

\[
\sigma_\star = \frac{ne^2}{m^*} = -ne\mu.
\]
and
\[ \mu \equiv \text{electron mobility} \]
\[ = (-e) \frac{<\tau>}{m*}. \quad (4-62) \]

The expression for averaging \(< (E) >\) is defined for any function of the energy, \(\gamma(E)\), by

\[ <\gamma(E)> = \frac{\int_{E_c}^{\infty} \gamma(E)(E-E_c)^{3/2} \frac{\partial f_\phi(E)}{\partial E} dE}{\int_{E_c}^{\infty} (E-E_c)^{3/2} \frac{\partial f_\phi(E)}{\partial E} dE} \quad (4-63) \]

It applies to Maxwell-Boltzmann as well as to Fermi-Dirac statistics.

The conductivity tensor coefficient \(\sigma_{ijk}\) for the spherical conduction band is given by

\[ \sigma_{ijk} = -\frac{ne^3}{m^*} <\tau^2> \zeta_{ijk}. \quad (4-64) \]

The magnetoconductivity tensor coefficient \(\sigma_{ijkl}\) is given for the case of spherical conduction band by

\[ \sigma_{ijkl} = -\frac{ne^4}{m^*} <\tau^3> \zeta_{ijkl}. \quad (4-65) \]
where \( \zeta_{ijkl} \) is defined by

\[
\zeta_{ijkl} = \frac{1}{2} (\epsilon_{ikm} \epsilon_{jkm} + \epsilon_{ilm} \epsilon_{jlm})
\]

(4-66)

with summation on the index \( m \). \( \zeta_{ijkl} \) has the following properties

\[
\begin{align*}
\zeta_{1111} &= \zeta_{2222} = \zeta_{3333} = 0 \\
\zeta_{1122} &= \zeta_{3311} = \zeta_{ijij} = 1 \quad \text{for } i \neq j \\
\zeta_{1212} &= \zeta_{2323} = \zeta_{ijij} = -\frac{1}{2} \quad \text{for } i \neq j \\
\zeta_{ijkl} &= \zeta_{jikl} = \zeta_{ijlk} = \zeta_{iklj}
\end{align*}
\]

4.5.2 Quadratic Energy Surfaces of the Many-Valley Type

For many semiconductors of cubic symmetry, the conduction band energy surfaces near the band edge points are ellipsoids of revolution, i.e. spheroids, centered around these points.

With one band edge point as centre and the ellipsoidal principal axes as coordinates, each ellipsoid could be represented by

\[
E = E_c + \hbar^2 \left[ \frac{K_1^2}{m_1} + \frac{K_2^2}{m_2} + \frac{K_3^2}{m_3} \right]
\]

(4-67)

If \( K_1 \) - axis is an axis of revolution, then

\[
m_2 = m_3
\]

(4-68)

and the effective mass ratio could be defined, as usual, by

\[
K = \frac{m_1}{m_3} = \frac{m_1}{m_2}
\]

(4-69)
The contribution of each such spheroid to the density of electron states is scalar and for D symmetrical spheroids the total density of electron states is

\[ L(E) = \frac{D}{2\pi^2} \frac{\sqrt{8 m_1 m_2 m_3}}{n^3} (E - E_C)^{1/2} \]  

(4-70)

\[ = \frac{1}{2\pi^2} \left[ \frac{2m_d}{\hbar^2} \right]^{3/2} (E - E_C)^{1/2} \]  

(4-71)

\[ = A (E - E_C)^{1/2} \]  

(4-72)

where \( L(E) \) is being expressed in the same form as that for spherical energy surfaces. In this form, the mass \( m_d \) is given by

\[ m_d = (D \frac{m_1 m_2 m_3}{2})^{1/3} \]  

(4-73)

\[ \equiv \] the density of states effective mass,

and

\[ A = \frac{1}{2\pi^2} \left[ \frac{2m_d}{\hbar^2} \right]^{3/2} = \frac{D}{2\pi^2} \frac{(8 m_1 m_2 m_3)^{1/2}}{n^3} \]  

(4-74)

The electron concentration for these D ellipsoids of the conduction band is given by

\[ n = \int_{E_C}^{\infty} L(E) f_o(E) \, dE \]

Two cases of spheroidal energy surfaces will be considered here:
i) 6 energy spheroids of main axes along \(<100>\) directions.
ii) 8 energy spheroids of main axes along \(<111>\) directions.

The conductivity tensor coefficients for these band structures could be determined as indicated in Section 4.4, the results are:

\[
\sigma_{ij} = \frac{ne^2 \langle \tau \rangle}{m_0} \delta_{ij},
\]

\[
\sigma_{ijk} = -\frac{ne^3 \langle \tau^2 \rangle}{m_0^2} \frac{3K(2+K)}{(1+2K)^2} \xi_{ijk},
\]

\[
\sigma_{1111} = -\frac{ne^4 \langle \tau^3 \rangle}{m_0^3} \lambda_{1111}(K),
\]

\[
\sigma_{1122} = -\frac{ne^4 \langle \tau^3 \rangle}{m_0^3} \lambda_{1122}(K),
\]

and

\[
\sigma_{1212} = -\frac{ne^4 \langle \tau^3 \rangle}{m_0^3} \lambda_{1212}(K),
\]

where \(\lambda_{1111}, \lambda_{1122}\) and \(\lambda_{1212}\) are functions of the effective mass ratio \(K\) which is defined by Equation (4-69). The full expressions of \(\sigma_{ij}, \sigma_{ijk}\) and \(\sigma_{ijkl}\) for these energy surfaces are written in Table (4-1). Also the corresponding expressions for the spherical band at (000)
are shown in this table. The quantity \( m_0 \) in the above equations is called the conductivity effective mass and, for spheroidal energy surfaces, is given by

\[
\frac{1}{m_0} = \frac{1}{3} \left[ \frac{1}{m_1} + \frac{1}{m_2} + \frac{1}{m_3} \right] \tag{4-80}
\]

\[
= \frac{1}{3} \frac{(1 + 2K)}{m_1} , \tag{4-81}
\]

where \( K = \frac{m_1}{m_2} = \frac{m_1}{m_3} \).

For spherical energy surfaces \( m_0 = m_1 = m_2 = m_3 \); and \( K = 1 \).

The resistivity tensor coefficients \( \rho_{ij} \) and \( \rho_{ijk} \) for the \((000)\) spherical surfaces, \(<100>\) spheroids and for the \(<111>\) spheroids, are given by:

\[
\rho_{ij} = \frac{m_0}{ne^2 <\tau>} \delta_{ij} \tag{4-82}
\]

\[
\rho_{ijk} = \frac{1}{ne} \frac{2}{<\tau>} \frac{3K(2+K)}{(1+2K)^2} \epsilon_{ijk} \tag{4-83}
\]

\[
= \rho_{123} \epsilon_{ijk}
\]

and if \( R_o \equiv \) Hall coefficient for small magnetic field,

\[
= -\rho_{123}
\]
then

\[ R_0 = -\frac{1}{ne} \frac{3K(2+K)}{\langle \tau \rangle^2 \langle \tau \rangle^2} \frac{1}{(1+2K)^2}. \] (4-84)

The magnetoresistivity tensor coefficients \( \gamma_{ijkl} \) are related to the magnetoconductivity tensor coefficients \( \sigma_{ijkl} \) by Equations (4-23) to (4-29).

The expressions of the conductivity and the resistivity tensor coefficients for the three energy surfaces configurations discussed here, are included in Table (4-1).

The condition of low magnetic field is

\[ \mu B \ll 1, \]

where \( \mu \) is the conductivity mobility = \( \frac{e\langle \tau \rangle}{m^*} \) in \( \frac{m^2}{\text{volt. sec}} \) and \( B \) is the magnetic field density in weber/m².

If the laboratory units of \( B \) in gauss and \( \mu \) in cm²/volt. sec are used, then the low magnetic field condition is:

\[ \mu B \times 10^{-8} \ll 1 \] (4-85)
<table>
<thead>
<tr>
<th>( f_i )</th>
<th>Spherical Surface</th>
<th>(&lt;100&gt; ) Ellipsoids</th>
<th>(&lt;111&gt; ) Ellipsoids</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \frac{1}{n^2} )</td>
<td>( \frac{1}{n} )</td>
<td>( \frac{1}{2} \left( \frac{1}{n_2^2} + \frac{1}{n_3^2} - \frac{1}{n_1^2} \right) )</td>
<td>( \frac{1}{2} \left( \frac{1}{n_2^2} + \frac{1}{n_3^2} - \frac{1}{n_1^2} \right) )</td>
</tr>
<tr>
<td>( \sigma_{11} )</td>
<td>( \frac{n^2 \sin \theta}{m - 4_{11}} )</td>
<td>( \frac{n^2 \sin \theta}{m} )</td>
<td>( \frac{n^2 \sin \theta}{m} )</td>
</tr>
<tr>
<td>( \sigma_{1j} )</td>
<td>( \frac{n^2 \sin \theta \cdot \sin \phi}{m} )</td>
<td>( \frac{n^2 \sin \theta \cdot \sin \phi}{m} )</td>
<td>( \frac{n^2 \sin \theta \cdot \sin \phi}{m} )</td>
</tr>
<tr>
<td>( \sigma_{1jk} )</td>
<td>( \frac{n^2 \sin \theta \cdot \sin \phi}{m} \cdot \langle 1j \rangle )</td>
<td>( \frac{3(2+K)}{m^2} )</td>
<td>( \frac{3(2+K)}{m^2} )</td>
</tr>
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<td>( \sigma_{1jk} )</td>
<td>( \frac{n^2 \sin \theta \cdot \sin \phi}{m} \cdot \langle 1j \rangle )</td>
<td>( \frac{3(2+K)}{m^2} )</td>
<td>( \frac{3(2+K)}{m^2} )</td>
</tr>
<tr>
<td>( \sigma_{111} )</td>
<td>( 0 )</td>
<td>( 0 )</td>
<td>( \frac{1}{m} \cdot \frac{1}{n} \cdot \langle 2 \rangle )</td>
</tr>
<tr>
<td>( \sigma_{112} )</td>
<td>( \frac{n \cdot \sin \phi}{m^2} )</td>
<td>( \frac{3(2+K)}{m^2} )</td>
<td>( \frac{3(2+K)}{m^2} )</td>
</tr>
<tr>
<td>( \sigma_{122} )</td>
<td>( \frac{n \cdot \sin \phi}{m^2} )</td>
<td>( \frac{3(2+K)}{m^2} )</td>
<td>( \frac{3(2+K)}{m^2} )</td>
</tr>
<tr>
<td>( \sigma_{111} )</td>
<td>( \frac{1}{m} \cdot \frac{1}{n} \cdot \langle 2 \rangle )</td>
<td>( \frac{1}{m} \cdot \frac{1}{n} \cdot \langle 2 \rangle )</td>
<td>( \frac{1}{m} \cdot \frac{1}{n} \cdot \langle 2 \rangle )</td>
</tr>
<tr>
<td>( \sigma_{112} )</td>
<td>( \frac{1}{m} \cdot \frac{1}{n} \cdot \langle 2 \rangle )</td>
<td>( \frac{1}{m} \cdot \frac{1}{n} \cdot \langle 2 \rangle )</td>
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</tr>
<tr>
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<td>( \frac{1}{m} \cdot \frac{1}{n} \cdot \langle 2 \rangle )</td>
<td>( \frac{1}{m} \cdot \frac{1}{n} \cdot \langle 2 \rangle )</td>
<td>( \frac{1}{m} \cdot \frac{1}{n} \cdot \langle 2 \rangle )</td>
</tr>
</tbody>
</table>
CHAPTER 5

ELECTRICAL TRANSPORT THEORY FOR GaAs$_{1-x}$P$_x$

In this chapter, the electrical transport theory will be further developed with special attention to applications in GaAs$_{1-x}$P$_x$.

5.1 Electrical Properties of a Cubic Semiconductor with Many Noninteracting Bands

Consider a cubic semiconductor of a band structure which consists of more than one set of spheroidal valleys. The low magnetic field conductivity expression, holds for each set of valleys as well as for the sets combined, since

\[ \sigma_{ij}(B) = \sigma_{ij} + \sigma_{ijk}B_k + \sigma_{ijkl}B_kB_l \] (5-1)

The \( n \)th set of valleys satisfies the cubic symmetry, therefore it has

\[ \sigma_{ij}^{(n)} = \sigma_0 \delta_{ij} \] (5-3)

and

\[ \sigma_{ijk}^{(n)} = \sigma_{123} \varepsilon_{ijk} \] (5-4)

and the independent coefficients of \( \sigma_{ijk}^{(n)} \) are \( \sigma_{1111}^{(n)} \), \( \sigma_{1122}^{(n)} \), and \( \sigma_{1212}^{(n)} \).

The conductivity tensor coefficients of this semiconductor could be expressed by
Since it is easier to measure the resistivity tensor coefficients in the laboratory, expressions relating the total resistivity tensor coefficient to individual sets tensor coefficients are desirable. The low magnetic field resistivity tensor for this semiconductor could be written as

\[ \rho_{ij} (B) = \rho_{ij} + \rho_{ijk} B_k + \rho_{ijkl} B_k B_l . \]  

These expressions will be derived below with the use of Equations (4-23) to (4-29).

Resistivity:

\[ \rho_{ij} = \rho_0 \delta_{ij} = \frac{1}{\sigma_0} \delta_{ij} \]  

\[ \sigma_0 = \sum_n \sigma_0^{(n)} \]  

\[ \frac{1}{\rho_0} = \sum_n \frac{1}{\rho_0^{(n)}} . \]  

Hall Coefficient:

\[ R_0 = -\rho_{123} = \frac{\sigma_{123}}{\sigma_0^2} = \text{Hall coefficient at zero magnetic field.} \]
\[ R_n^{(n)} = - \rho_{123}^{(n)} = \frac{\sigma^{(n)}}{[\sigma^{(n)}]^2} = n^{th} \text{ band Hall coefficient at zero magnetic field.} \] (5-13)

Then
\[ \frac{R_o}{\rho_o^2} = \sum_n \frac{R^{(n)}}{[\rho_o^{(n)}]^2} = \sum_n \frac{\rho_{123}^{(n)}}{[\rho_o^{(n)}]^2} \] (5-14)

or
\[ R_o \rho_o^2 = \sum_n R^{(n)} [\sigma^{(n)}]^2 \] (5-15)

Magnetoresistivity Coefficients:

i) \[ \sigma_{1111} = - \frac{\rho_{1111}}{\rho_o^2} = \sum_n \sigma^{(n)} \] (5-16)

then
\[ \frac{\rho_{1111}}{\rho_o^2} = \sum_n \frac{\rho^{(n)}_{1111}}{[\rho_o^{(n)}]^2} \] (5-17)

ii) \[ - \sigma_{1122} = \frac{\rho_{1122}}{\rho_o^2} + \frac{\rho_{123}^2}{\rho_o^3} = - \sum_n \sigma^{(n)}_{1122} \] (5-18)

then
\[ \frac{\rho_{1122}}{\rho_o^2} + \frac{\rho_{123}^2}{\rho_o^3} = \sum_n \left\{ \frac{\rho^{(n)}_{1122}}{[\rho_o^{(n)}]^2} + \frac{[\rho_{123}^{(n)}]^2}{[\rho_o^{(n)}]^3} \right\} \] (5-19)

iii) \[ 2\sigma_{1212} = - \frac{2\rho_{1212}}{\rho_o^2} + \frac{\rho_{123}^2}{\rho_o^3} = \sum_n 2\sigma^{(n)}_{1212} \] (5-20)
\[
\text{then } \frac{2p_{1212}}{\rho_o} + \frac{2p_{123}}{\rho_o^3} = \sum_n \left\{ -\frac{2p_{1212}}{[\rho_o^{(n)}]^2} + \frac{[\rho_{123}^{(n)}]^2}{[\rho_o^{(n)}]^3} \right\}. \quad (5-21)
\]

And from Equations (16) to (21), it could be seen that

\[
\frac{\rho_{1111} + \rho_{1122} + 2\rho_{1212}}{\rho_o^2} = - (\sigma_{1111} + \sigma_{1122} + 2\sigma_{1212})
\]

\[
= - \sum_n \left[ \sigma_{1111}^{(n)} + \sigma_{1122}^{(n)} + 2\sigma_{1212}^{(n)} \right] \]

\[
= \sum_n \frac{\rho_{1111}^{(n)} + \rho_{1122}^{(n)} + 2\rho_{1212}^{(n)}}{[\rho_o^{(n)}]^2}. \quad (5-22)
\]

5.2 Hall Coefficient and Conductivity of a Two-Band Cubic Semiconductor

For a semiconductor having more than one type of charge carrier; e.g. holes and electrons, or electrons belonging to different conduction bands and thus acquiring different mobilities, the Hall coefficient and the conductivity will depend on the magnetic field even if they are independent of that field for each type of carriers.
Figure (5-1). Components of electric field and current for a sample made out of (100) wafer.

Figure (5-2). Coordinate systems for a sample cut out of (100) wafer.
With application to the case of GaAs$_{1-x}$Px in mind, the Hall coefficient and conductivity of a two-band cubic semiconductor will be discussed here. The discussion will be limited to samples cut from (100) wafers since this is the surface orientation of most of the samples used here.

Consider a coordinate system made of the cubic axes. Figure (5-1) shows a sample cut from a (100) wafer with its length making an angle $\psi$ with the [100] axis. The current density will be

$$J = (J_1, J_2, 0) = (J \cos \psi, J \sin \psi, 0) \quad (5-23)$$

The relations between the current density components ($J_1, J_2$) and the electric field components ($E_1, E_2$) could be written as

$$J_1 = \sigma_{11}(B) E_1 + \sigma_{12}(B) E_2 \quad (5-24)$$

and

$$J_2 = \sigma_{21}(B) E_1 + \sigma_{22}(B) E_2 \quad (5-25)$$

where $\sigma_{ij}(B) \equiv \sigma_{ij}(B) = \sigma_{ij}(B_1, B_2, B_3) = \text{the conductivity tensor.}$

These equations could also be written as

$$E_1 = \rho_{11}(B) J_1 + \rho_{12}(B) J_2 \quad (5-26)$$

$$E_2 = \rho_{21}(B) J_1 + \rho_{22}(B) J_2 \quad (5-27)$$

where elements of $\rho_{ij}(B)$, the resistivity tensor, are related to elements of $\sigma_{ij}(B)$ by

$$\rho_{11}(B) = \frac{\sigma_{22}(B)}{\Delta} \quad (5-28)$$
\[ \rho_{22}(B) = \frac{\sigma_{11}(B)}{\Delta}, \quad (5-29) \]

\[ \rho_{12}(B) = -\frac{\sigma_{12}(B)}{\Delta}, \quad (5-30) \]

\[ \rho_{21}(B) = -\frac{\sigma_{21}(B)}{\Delta}, \quad (5-31) \]

and

\[ \Delta = \sigma_{11}(B)\sigma_{22}(B) - \sigma_{12}(B)\sigma_{21}(B) \quad (5-32) \]

In the following subsections, the cases of transverse and longitudinal magnetic field will be considered separately.

5.2.1 Transverse Magnetic Field

Consider Figure (5-1) with the magnetic field \( B = (0, 0, B) \).

The conductivity and resistivity tensor elements will have

\[ \sigma_{11}(B) = \sigma_{22}(B) \],

\[ \sigma_{12}(B) = -\sigma_{21}(B) \],

and

\[ \rho_{11}(B) = \rho_{22}(B) = \frac{\sigma_{22}(B)}{\Delta_t} \],

\[ \rho_{12}(B) = -\rho_{21}(B) = -\frac{\sigma_{12}(B)}{\Delta_t} \],

where

\[ \Delta_t = \sigma_{11}^2(B) + \sigma_{12}^2(B) \quad (5-35) \]

The components of the electric field along and transverse to the sample could be written as
\[ E_L = E_1 \cos \psi + E_2 \sin \psi , \]

and \[ E_T = -E_1 \sin \psi + E_2 \cos \psi . \]  

Using Equations (5-23), (5-26), (5-27) with the above equations, then

\[ E_L = \rho_{11}(B) J = \frac{J}{\sigma(B)} , \]  

and

\[ E_T = \rho_{21}(B) J = R(B) BJ . \]  

Equation (5-37) defines the conductivity \( \sigma(B) \) as it is being measured in the laboratory, i.e. the ratio of the current density to the electric field along this current. And Equation (5-38) defines the Hall coefficient \( R(B) \).

So, for a cubic semiconductor in a transverse magnetic field, the values of the conductivity and Hall coefficient for the sample shown in Figure (5-1), of any angle \( \psi \), are given by

\[ \sigma(B) = \frac{\sigma_{11}^2(B) + \sigma_{12}^2(B)}{\sigma_{11}(B)} = \frac{\Delta t}{\sigma_{11}(B)} , \]  

and

\[ R(B) = \frac{1}{B} \frac{\sigma_{12}(B)}{\sigma_{11}^2(B) + \sigma_{12}^2(B)} = \frac{\sigma_{12}(B)}{B \Delta t} . \]  

For the case of a semiconductor having two uncoupled energy bands, the conducting components can be written as the sums of contributions from each band.

\[ \sigma_{ij}(B) = \sigma_{ij}^{(1)}(B) + \sigma_{ij}^{(2)}(B) . \]  

And Equations (5-39) and (5-40) for \( \sigma(B) \) and \( R(B) \) hold again for this two-band semiconductor.
Let the conductivity and Hall coefficient for the first band be \( \sigma(1) \) and \( R(1) \) respectively. And for the second band let the conductivity and Hall coefficient be \( \sigma(2) \) and \( R(2) \).

From Equations (5-39) and (5-40) applied to each band separately, it could be seen that

\[
\frac{\sigma_{12}(B)}{\sigma_{11}(B)} = R(i) \sigma(i) B, \quad (5-42)
\]

\[
\sigma_{11}(B) = \frac{\sigma(i)}{1 + \sigma(i) R(i) B^2}, \quad (5-43)
\]

and

\[
\sigma_{12}(B) = \frac{\sigma(i) R(i) B}{1 + \sigma(i) R(i) B^2}, \quad (5-44)
\]

for \( i = 1 \) or 2

Now it is possible, by using the above equations together with Equation (5-41), to get expressions for \( \sigma_{11}(B) \) and \( \sigma_{12}(B) \) of the two-band semiconductor in terms of the conductivity and Hall coefficient of each band. In turn, these equations could be used to obtain expressions for \( \sigma(B) \) and \( R(B) \) of this two-band semiconductor. The results of these algebraic steps are

\[
\Delta_t = \sigma_{11}^2(B) + \sigma_{12}^2(B) = \frac{\left[\sigma(1) + \sigma(2)\right]^2 + \sigma(1) \sigma(2) \left[R(1) + R(2)\right]^2 B^2}{\left[1 + \sigma(1) R(1) B^2\right] \left[1 + \sigma(2) R(2) B^2\right]}, \quad (5-45)
\]
\[
\sigma(B) = \frac{\left[\sigma(1) + \sigma(2)\right]^2 + \sigma(1)^2 \sigma(2)^2 \left[R(1) + R(2)\right]^2 B^2}{\left[\sigma(1) + \sigma(2)\right] + \sigma(1)^2 \sigma(2)^2 \left[R(1)^2 + \sigma(2)^2 R(2)^2\right] B^2},
\]

(5-46)

\[
\rho(B) \equiv \text{resistivity} = \frac{1}{\sigma(B)},
\]

(5-47)

and

\[
R(B) = \frac{R(1)^2 + R(2)^2}{\left[\sigma(1) + \sigma(2)\right]^2 + \sigma(1)^2 \sigma(2)^2 \left[R(1)^2 + \sigma(2)^2 R(2)^2\right] B^2}.
\]

(5-48)

These equations have been mentioned in many references.

From their derivation, it could easily be seen that the two bands could have spherical or ellipsoidal surfaces or any other shape with any number of minima or maxima. The magnetic field in this derivation was assumed to be transverse to (100) plane and to have any value.

The value of the magnetic field used in this research is small and these equations could be written again neglecting terms of \(B^4\) or higher order dependence. The following approximations will result:

\[
\sigma(B) \approx \left[\sigma(1) + \sigma(2)\right] - \frac{\sigma(1) \sigma(2)}{\left[\sigma(1) + \sigma(2)\right]^2} \left[R(1) - \sigma(2) R(2)\right] B^2,
\]

(5-49)

\[
\rho(B) = \frac{\sigma(1) \sigma(2)}{\left[\sigma(1) + \sigma(2)\right]^3} \left[R(1) - \sigma(2) R(2)\right] B^2,
\]

(5-50)

and
Equations (5-49), (5-50) and (5-51) show that for a cubic semiconductor of two uncoupled energy bands and in a small magnetic field, the magnitude of the conductivity and Hall coefficient decreases as the magnetic field is increased, while the magnitude of the resistivity increases with the increase of the magnetic field. The changes in these quantities are given by the second term in each equation. This change is proportional to the square of the algebraic difference between the mobilities of the charge carriers in each band, and it will be zero if the semiconductor has one band only because the conductivity of the other band will be zero. The first term in these equations could also be dependent on the magnetic field.

The above equations could also be derived more readily by the use of the conductivity and resistivity tensor coefficients which are given at small magnetic field by

\[ \sigma_{ij}^{(B)} = \sigma_0 \delta_{ij} + \sigma_{123}^{\xi} ijk B_k + \sigma_{ijk} B_k B_\xi \]

and

\[ \rho_{ij}^{(B)} = \rho_0 \delta_{ij} + \rho_{123}^{\xi} ijk B_k + \rho_{ijk} B_k B_\xi \]

Similar expressions apply for each band separately.
For \( B = (0, 0, B) \), the conductivity tensor elements \( \sigma_{11}(B) \) and \( \sigma_{12}(B) \) of this cubic semiconductor could be written as
\[
\sigma_{11}(B) = \sigma_0 + \sigma_{1133} B^2 ,
\]
(5-52)
and
\[
\sigma_{12}(B) = \sigma_{123} B .
\]
(5-53)

Also, for each band, these quantities are
\[
\sigma^{(i)}_{11}(B) = \sigma^{(i)}_0 + \sigma^{(i)}_{1133} B^2 ,
\]
(5-54)
and
\[
\sigma^{(i)}_{12}(B) = \sigma^{(i)}_{123} B ,
\]
(5-55)
for \( i = 1 \) or \( 2 \).

So, for this two-band semiconductor, the conductivity, resistivity and Hall coefficient for small magnetic field are
\[
\sigma(B) = \sigma_{11}(B) + \frac{\sigma_{12}^2(B)}{\sigma_{11}(B)} = \left[ \sigma^{(1)}_0 + \sigma^{(2)}_0 \right] + \left[ \sigma^{(1)}_{1133} + \sigma^{(2)}_{1133} \right] B^2 + \frac{\left[ \sigma^{(1)}_{123} + \sigma^{(2)}_{123} \right]^2}{\sigma^{(1)}_0 + \sigma^{(2)}_0} B^2 ,
\]
(5-56)
\[
\rho(B) = \frac{1}{\sigma(B)} = \frac{1}{\left[ \sigma^{(1)}_0 + \sigma^{(2)}_0 \right]} - \frac{\left[ \sigma^{(1)}_{1133} + \sigma^{(2)}_{1133} \right]}{\left[ \sigma^{(1)}_0 + \sigma^{(2)}_0 \right]^2} B^2 - \frac{\left[ \sigma^{(1)}_{123} + \sigma^{(2)}_{123} \right]^2}{\left[ \sigma^{(1)}_0 + \sigma^{(2)}_0 \right]^3} B^2 ,
\]
(5-57)
and
\[ R(B) = \frac{\sigma_{12}(B)}{B[\sigma_{11}^2(B) + \sigma_{12}^2(B)]} \]
\[ = \frac{\sigma_{123}}{\sigma_0^2} \left\{ 1 - \frac{2\sigma_{1133}}{\sigma_0} B^2 - \frac{\sigma_{123}^2}{\sigma_0^2} B^2 \right\} \]
\[ = R_0 - R_0 \left\{ \frac{2\rho\sigma_{1133}}{\sigma_0^2} + \frac{R_0^2}{\sigma_0^2} \right\} B^2, \quad (5-58) \]

or
\[ R(B) = R_0 - R_0 \left\{ 2\rho\sigma_{1133} + \frac{R_0^2}{\sigma_0^2} \right\} B^2, \quad (5-59) \]

where
\[ R_0 = \frac{\sigma_{123}}{\sigma_0^2} = \frac{\sigma(1)}{\sigma_0^2} + \frac{\sigma(2)}{\sigma_0^2} = \frac{\sigma(1)}{\sigma_0} + \frac{\sigma(2)}{\sigma_0} \]
\[ \frac{\sigma_{1133}}{\sigma_0^2} = \frac{\rho}{\sigma_0^2} \left[ \frac{\sigma(1)}{\sigma_0} + \frac{\sigma(2)}{\sigma_0} \right] \]

and
\[ \sigma_0 = \sigma_0(1) + \sigma_0(2) . \]

It could be easily shown that these expressions are the same as those given previously by Equations (5-49), (5-50), and (5-51).

5.2.2 Longitudinal Magnetic Field along [110] direction:

For the case when \( B \) is along the length of the sample shown in Figure (5-1) and \( \psi = \frac{\pi}{4} \), then
\[ B = \left( \frac{B}{\sqrt{2}}, \frac{B}{\sqrt{2}}, 0 \right) . \]
The conductivity tensor elements will have the relations

\[ \sigma_{11}(B) = \sigma_{22}(B) \quad (5-61a) \]

and

\[ \sigma_{12}(B) = \sigma_{21}(B) \quad . \quad (5-61b) \]

These relations could easily be derived by using the tensor
transformation rule

\[ \sigma_{ij}(B', B', B') = a_{ik} a_{jl} \sigma_{kl}(B_1, B_2, B_3) \quad , \quad (5-62a) \]

where

\[ B'_i = |a| a_i B_j \quad , \quad (5-62b) \]

for \(|a| = [a_3] = \) matrix representing reflection in (110) plane.

The resistivity tensor elements could be obtained from

Equations (5-28) and (5-31)

\[ \rho_{11}(B) = \rho_{22}(B) = \frac{\sigma_{11}(B)}{\Delta_L} \quad , \quad (5-63a) \]

and

\[ \rho_{21}(B) = -\frac{\sigma_{21}(B)}{\Delta_L} = \rho_{12}(B) \quad , \quad (5-63b) \]

where \( \Delta_L = \sigma_{11}(B) - \sigma_{12}(B) \quad . \quad (5-64) \)

From Equations (5-26), (5-27), (5-36) and (5-63), the expressions for \( E_L \) and \( E_T \) are
\[ E_L = \rho_{11}(B) J + \rho_{12}(B) J \sin 2 \psi \]

and

\[ E_T = \rho_{12}(B) J \cos 2 \psi \]

For \( \psi = \frac{\pi}{4} \), these equations yield

\[ E_L = \left[ \rho_{11}(B) + \rho_{12}(B) \right] J = \frac{J}{\sigma_\parallel(B)} \quad , \]

and

\[ E_T = 0 \quad . \]

This defines the longitudinal conductivity \( \sigma_\parallel(B) \) as

\[ \sigma_\parallel(B) = \frac{1}{\rho_{11}(B) + \rho_{12}(B)} = \frac{\Delta_\parallel}{\sigma_{11}(B) - \sigma_{21}(B)} \]

\[ = \sigma_{11}(B) + \sigma_{12}(B) \quad , \]

where the definition of \( \Delta_\parallel \) was used for last equation.

For the two band semiconductor

\[ \sigma_\parallel(B) = \sigma_{11}(B) + \sigma_{12}(B) \quad (5-69) \]

\[ = \sigma_{11}^{(1)}(B) + \sigma_{11}^{(2)}(B) + \sigma_{12}^{(1)}(B) + \sigma_{12}^{(2)}(B) \quad (5-70) \]

\[ = \sigma_\parallel^{(1)}(B) + \sigma_\parallel^{(2)}(B) \quad . \]

These equations show that, in a longitudinal magnetic field along [110] and of any value, the conductivity of this two-band semiconductor is equal to the sum of the conductivities of each band; and as seen from Equations (5-70) and (5-71), there is no additional terms, as in Equation (5-49), mixing the two bands.
For small magnetic field \( B = \left( \frac{B}{\sqrt{2}}, \frac{B}{\sqrt{2}}, 0 \right) \), the conductivity elements \( \sigma_{11}(B) \) and \( \sigma_{12}(B) \) could be written as

\[
\sigma_{11}(B) = \sigma^0 + \left( \sigma_{1111} + \sigma_{1122} \right) \frac{B^2}{2}, \quad \text{(5-72)}
\]

and

\[
\sigma_{12}(B) = \sigma_{1212} B^2. \quad \text{(5-73)}
\]

So for this cubic two-band semiconductor in a longitudinal small magnetic field along [110], the conductivity is given by

\[
\sigma_{\parallel}(B) = \sigma^0(1) + \sigma^0(2) + \frac{1}{2} \sigma_{1111}(1) + \frac{1}{2} \sigma_{1122}(1) + \sigma_{1212}(1) B^2 \\
+ \frac{1}{2} \sigma_{1111}(2) + \frac{1}{2} \sigma_{1122}(2) + \sigma_{1212}(2) B^2. \quad \text{(5-74)}
\]

5.3 Determination of Seitz Magnetoresistance Coefficients

5.3.1 For samples made of (100) wafers

In this research most of the samples used were made of wafers of (100) surfaces. Their lengths were cut along <100> or <110> directions.

Consider a rectangular coordinate system \((x, y, z)\) made of the main cubic crystal axes. And assume that the sample was cut such that its length makes an angle \( \psi \) with the [100] axis and then it is placed in a magnetic field \( B \).

Consider another frame of rectangular coordinates \((x_1, y_1, z_1)\) attached to the sample as shown in Figure (5-2).
Let $\theta, \delta, \phi$ be the angles between the magnetic field and the sample length, width and thickness respectively. The thickness is always along z-direction.

Referred to the crystal axes, the direction cosines of the current i.e. sample length are $(l_1, l_2, l_3) = (\cos \psi, \sin \psi, 0)$ and the direction cosines of the magnetic field are

$$(n_1, n_2, n_3) = [(\cos \theta \cos \psi - \cos \delta \sin \psi),$$

$$(\cos \theta \sin \psi + \cos \delta \cos \psi),$$

$$\cos \phi]. \quad (5-75)$$

In preparation for evaluating the magnetoresistance $\frac{\Delta \rho}{\rho_o B^2}$, it is seen

$$\sum l_i n_i = \cos \theta, \quad (5-76)$$

$$\sum l_i n_i^2 = \cos^2 \theta - \frac{1}{2} \sin^2 2\psi (\cos^2 \theta - \cos^2 \delta)$$

$$- \frac{1}{2} \sin 4\psi \cos \theta \cos \delta. \quad (5-77)$$

So, $\frac{\Delta \rho}{\rho_o B^2}$, which is given by Equation (4-40) of Chapter IV, could be written as

$$\frac{\Delta \rho}{\rho_o B^2} = b + (c + d) \cos^2 \theta$$

$$- \frac{1}{2} d \sin^2 2\psi [\cos^2 \theta - \cos^2 \delta]$$

$$- \frac{1}{2} d \sin 4\psi \cos \theta \cos \delta. \quad (5-78)$$
The angle $\psi$ is fixed by the cutting of the sample. Considering the two possibilities of orienting the sample length:

$\psi = 0$ and $\psi = 45^\circ$,

it was preferred to cut most of the samples such that $\psi = 45^\circ$, since this would allow the inclusion of more terms in the last equation to be able to determine Seitz magnetoresistance coefficients $b$, $c$ and $d$.

For $\psi = 45^\circ$, we have

$$\frac{\Delta \rho}{\rho_0 B^2} = b + (c + d) \cos^2 \theta$$

$$- \frac{1}{2} d [\cos^2 \theta - \cos^2 \phi]. \quad (5-79)$$

In experiment, the sample is placed in the magnetic field and rotated with the length making an angle $\theta$ with that field. In this case there are two configurations:

1. $\mathbf{B}$ could always be perpendicular to the sample width, i.e., $\phi = 90^\circ$; then

$$\frac{\Delta \rho}{\rho_0 B^2} = b + (c + \frac{1}{2} d) \cos^2 \theta, \quad (5-80)$$

or

2. $\mathbf{B}$ could always be perpendicular to sample thickness, i.e. $\mathbf{B}$ has no component in the $z$-direction, in which case the angle $\phi = 90^\circ$ and $\phi + \theta = 90^\circ$, then

$$\frac{\Delta \rho}{\rho_0 B^2} = (b + \frac{1}{2} d) + c \cos^2 \theta. \quad (5-81)$$
Thus with one sample only cut from a wafer of (100) surface such that its length is along the direction [110], it is possible to get the coefficients $b$, $c$ and $d$. For this purpose, the sample should be placed in the above two configurations. From the first configuration, $b$ and $(c + \frac{1}{2} d)$ could be obtained. From the second configuration $(b + \frac{1}{2} d)$ and $c$ could be obtained. So Seitz magnetoresistance coefficients $a$, $b$ and $d$ could be determined to check the energy band structure for the semiconductor as will be shown below.

5.3.2 For samples made of (111) wafers

In the case of a wafer of (111) surface, one sample in one configuration is enough to determine these coefficients. The sample thickness will be along [111] direction and it could be ultrasonically cut such that its length is along [112] direction. Then

$$(\ell_1, \ell_2, \ell_3) = \left( \frac{1}{\sqrt{6}}, \frac{1}{\sqrt{6}}, \frac{-2}{\sqrt{6}} \right).$$

And the perpendicular to sample surface will have the direction cosines

$$(t_1, t_2, t_3) = \left( \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}} \right).$$

In this configuration, the magnetic field will always be perpendicular to sample width and if $\alpha$ is the angle between this field and sample length, then relative to crystal cubic axes the magnetic field will have the direction cosines:
\[ \eta_1 = \frac{1}{\sqrt{6}} \cos \theta + \frac{1}{\sqrt{3}} \sin \theta \]
\[ \eta_2 = \frac{1}{\sqrt{6}} \cos \theta + \frac{1}{\sqrt{3}} \sin \theta \]
\[ \eta_3 = -\frac{2}{\sqrt{6}} \cos \theta + \frac{1}{\sqrt{3}} \sin \theta . \]

Then
\[ \sum \eta \cdot \eta = \cos \theta , \]
and
\[ \sum \eta^2 \cdot \eta = \frac{1}{2} \cos^2 \theta + \frac{1}{3} \sin^2 \theta - \frac{1}{3\sqrt{2}} \sin 2 \theta . \]

From Equation (4-40) of Chapter IV, the magnetoresistance at
\[ \theta = 0, \quad \theta = 45^\circ \quad \text{and} \quad \theta = 90^\circ \]
will be given respectively by
\[ \frac{\Delta \rho}{\rho_0 B^2} \bigg|_{\theta = 0} = b + c + \frac{1}{2} d , \quad (5-82) \]
\[ \text{at } \theta = 0^\circ \]
\[ \frac{\Delta \rho}{\rho_0 B^2} \bigg|_{\theta = 45^\circ} = b + \frac{1}{2} c + \left( \frac{5}{12} - \frac{1}{3\sqrt{2}} \right) d , \quad (5-83) \]
\[ \text{at } \theta = 45^\circ \]
and
\[ \frac{\Delta \rho}{\rho_0 B^2} \bigg|_{\theta = 90^\circ} = b + \frac{1}{3} d \quad (5-84) \]
\[ \text{at } \theta = 90^\circ \]

The coefficients \( b, c \) and \( d \) could be determined from these equations.
5.3.3 Some Notes about Seitz Magnetoresistance Coefficients

The units to be used for evaluating $\frac{\Delta \rho}{\rho_0 B^2}$ or the Seitz magnetoresistance coefficients $b$, $c$ and $d$ could be different from the M.K.S. units which has the weber/m$^2$ as the magnetic field density unit.

If the magnetic field density is $B_1$ Kilogauss, then

$$B = B_1 \text{ K Gauss} = \frac{B_1}{10} \text{ weber/m}^2,$$

and

$$\frac{\Delta \rho}{\rho_0 B^2} = \frac{\Delta \rho}{\rho_0} \frac{100}{B^2} \text{ m}^4/\text{weber}^2,$$

$$= \frac{\Delta \rho}{\rho_0} \frac{10}{B_1^2} \text{ cm}^4/\text{volt}^2 \text{ sec}^2 \quad (5-85)$$

Seitz magnetoresistance coefficients $b$, $c$ and $d$ could be obtained in units of cm$^4$/volt$^2$ sec$^2$ if $\frac{\Delta \rho}{\rho_0 B^2}$ is expressed by the last equation.

The energy band structure could be inferred from these coefficients. Under the assumption of the existence of a relaxation time, the symmetry of the energy surfaces imposes the following conditions:

for (000) spheres, $b + c = 0$ and $d = 0$, \hspace{1cm} (5-86)

for <100> spheroids, $b + c + d = 0$ and $d < 0$, \hspace{1cm} (5-87)
for \(<111>\) spheroids, \(b + c = 0\) and \(d > 0\), \(5-88\)

and for \(<110>\) spheroids \(b + c = d\) and \(d > 0\). \(5-89\)

These relations could be easily arrived at by using the definitions of \(b\), \(c\) and \(d\), as given by Equations (4-37), (4-38) and (4-39) of Chapter IV, together with the values \(p_{ijkl}\) for each of the energy surfaces given by Table (4-1). While these relations are based on the assumption of a relaxation time, they are independent of the scattering mechanism. So far, there has been no indication of their validity at conditions where the relaxation time loses its meaning.

5.4 Electrical Properties of GaAs<sub>1-x</sub>P<sub>x</sub> Considering Two Conduction Bands.

In this section, the electrical properties of n-type GaAs<sub>1-x</sub>P<sub>x</sub> will be considered. The conduction band will be assumed to contain two subbands:

1) The first subband, which consists of the spherical valley at \((000)\).

2) The second subband, which consists of 6 spheroidal valleys along \(<100>\) axes.
The quantities associated with the first subband will have the subscript 1 or \( a \). And those associated with the second subband will have the subscript 2 or \( b \). Subscripts \( a \) and \( b \) will be used wherever confusion with the tensor indices might arise. The subscript \( \circ \) will be used to indicate quantities at zero magnetic field.

At zero magnetic field, the conductivity and resistivity will be given by

\[
\sigma_{ij} = \sigma_0 \delta_{ij} = (\sigma_0^a + \sigma_0^b) \delta_{ij},
\]

and

\[
\rho_{ij} = \rho_0 \delta_{ij} = \frac{1}{\sigma_0} \delta_{ij},
\]

where

\[
\sigma_0 = \sigma_0^a + \sigma_0^b
\]

\[
= \frac{n_1 e^{2 <\tau_1>}}{m_1} + \frac{n_2 e^{2 <\tau_2>}}{m_2},
\]

\[
= -e (n_1 \nu_1 + n_2 \nu_2),
\]

and \( m_1, m_2 \) are the conductivity effective masses of the two subbands as given by Equation (4-80).
Also, at zero magnetic field, the Hall coefficient $R_0$ is related to $R_{o_a}$ and $R_{o_b}$ by Equation (5-60), namely

$$R_{o_0}^2 = R_{o_a}^2 + R_{o_b}^2$$

$$= \frac{n_1 e^2}{m_1^2} \tau_1^2 - \frac{n_2 e^2}{m_2^2} \tau_2^2 \frac{3K(2 + K)}{(1 + 2K)^2}$$

or

$$R_0 = \frac{R_{o_a}^2 + R_{o_b}^2}{(\sigma_{o_a} + \sigma_{o_b})^2} \quad (5-91)$$

The magnetoresistivity tensor coefficients, obtained from Equations (5-17), (5-18) and (5-20), could be written as

i) $\frac{\rho_{1111}}{\rho_o} = \frac{\rho_{1111a}}{\rho_{o_a}} + \frac{\rho_{1111b}}{\rho_{o_b}} \quad (5-92)$

$$= 0 + 0 \quad \text{for this case},$$

ii) $\frac{\rho_{1122}}{\rho_o} = -\frac{\rho_{123}^2}{\rho_o^3} - \sigma_{1122a} - \sigma_{1122b} \quad (5-93)$

$$= -R_o \sigma_{12} - \sigma_{1122},$$

and

iii) $\frac{\rho_{1212}}{\rho_o^2} = -\frac{\rho_{123}^2}{\rho_o^3} + 2\sigma_{1212a} + 2\sigma_{1212b} \quad (5-94)$

$$= -R_o^2 \sigma_{12} + 2\sigma_{1212}.$$
From the Seitz magnetoresistance coefficients, it is seen that

\[ b + c + \frac{1}{2} d = \frac{\rho_{1111} + \rho_{1122} + 2\rho_{1212}}{2\rho_o} \]

\[ = -\frac{1}{2} [\sigma_{1111} + \sigma_{1122} + 2\sigma_{1212}] . \]

But for the (000) valley, \( \sigma_{1111} + \sigma_{1122a} + 2\sigma_{1212a} = 0 \), and for the <100> valleys \( \sigma_{1111b} = 0 \), then

\[ b + c + \frac{1}{2} d = -\frac{1}{2\rho_o} [\sigma_{1122b} + 2\sigma_{1212b}] , \quad (5-95) \]

or

\[ \frac{1}{\rho_o} [b + c + \frac{1}{2} d] = \frac{n_2 e^4}{2 m^{3/2}_2} \langle \tau \rangle \frac{9K(K - 1)^2}{(1 + 2K)^3} , \quad (5-96) \]

where \( K \) is the effective mass ratio of the <100> spheroids. The quantity in the right side of this equation is a function of the <100> parameters only. It is not a function of the (000) valley.

As shown in Section 5.3, the quantity \( [b + c + \frac{1}{2} d] \) is given by \( \frac{\Delta \rho}{\rho_o B^2} \) when the magnetic field is along the sample length. Equation (5-96) shows that this quantity could be used to check the sphericity of the <100> valleys. Assuming the relaxation time to be isotropic and \( n_2 \neq 0 \), if \( [b + c + \frac{1}{2} d] = 0 \) then \( K = 1 \).
Also from Seitz magnetoresistance coefficient $b$, given by

$$b = \frac{\sigma_{1122}}{\rho_o} = - \frac{2\sigma_2}{\rho_o} - \frac{\sigma_{1122}}{\sigma_o} ,$$

then

$$\frac{1}{\rho_o} [b + \frac{2\sigma_2}{\rho_o}] = - \sigma_{1122} = - \sigma_{1122a} - \sigma_{1122b}$$

$$= \frac{n_1 e^4}{m_1^3} \langle \tau_1^{<3} \rangle + \frac{n_2 e^3}{m_2^3} \langle \tau_2^{<3} \rangle \frac{9K(1+K+K^2)}{(1+2K)^3}$$ (5-97)

where $R_o \sigma_o = \mu_H$, the Hall mobility.

From Equations (5-96) and (5-97), it is seen that

$$\frac{b + c + \frac{1}{2}d}{b + \frac{2}{\mu_H}} = \frac{2[\sigma_{1122a} + \sigma_{1122b}]}{\sigma_{1122b} + 2\sigma_{1122b}} ,$$

$$= \frac{(K-1)^2}{2 \frac{n_1 \langle \tau_1^{<3} \rangle}{m_1^3} \frac{m_2^{2\sigma}}{n_2 \langle \tau_2^{<3} \rangle} \frac{(1+2K)^3}{9K} + 2(1 + K + K^2)}$$ (5-98)

For GaP or GaAs $P$ of $x$ high enough, it will be possible if the ratio $\frac{n_1}{n_2} = 0$, to neglect the first term in denominator of the right side of this equation which makes it possible to determine $K$ in this case.
5.5 A Method for the Determination of Electron Density in Each Band and their Mobility Ratio

It was shown previously that Hall coefficient varies with the magnetic field according to the equation

$$R(B) = \frac{R_1\sigma_1^2 + R_2\sigma_2^2 + \sigma_1\sigma_2 R_1R_2 [R_1 + R_2] B^2}{(\sigma_1 + \sigma_2)^2 + \sigma_1^2\sigma_2^2 (R_1 + R_2)^2 B^2}$$

which is valid for any magnetic field and applies to the case of two noninteracting bands.

If the factors in $R_1$ and $R_2$ which depend on the scattering mechanism are taken to be unity, and if the energy surfaces of the two bands are assumed spherical, then

$$R_1 = -\frac{1}{n_1e} \quad \text{and} \quad R_2 = -\frac{1}{n_2e}$$

$$\sigma_1 = -en_1\mu_1 \quad \text{and} \quad \sigma_2 = -en_2\mu_2$$

(5-100)

where $e$ is the magnitude of the electronic charge.

For the purpose of this discussion on GaAs$_{1-x}$P$_x$, let $n_1$, $\mu_1$ be the density and mobility of electrons in the (000) valley and $n_2$, $\mu_2$ be the density and mobility of electrons in the <100> valleys. The equation for $R(B)$ could then be written as

$$R(B) = -\frac{1}{e} \frac{n_1\mu_1^2 + n_2 + \mu_1^2 (n_1 + n_2) B^2}{(n_1\mu_1 + n_2)^2 + \mu_1^2(n_1 + n_2)^2 B^2}$$

(5-101)

where $w = \frac{\mu_1}{\mu_2}$. 
In the limit of zero magnetic field, Hall coefficient is

\[ R_0 = -\frac{1}{e} \frac{n_1 w + n_2}{(n_1 w + n_2)^2} \]  

(5-102)

For small magnetic fields, the expression \( R(B) \) could be written as

\[ R(B) = R_0 + \frac{1}{e} \frac{(w-1)^2 \mu_1^2 n_1 n_2 (n_1 + n_2)}{(n_1 w + n_2)^4} B^2 \]  

(5-103)

where terms of \( B^4 \) or higher order terms have been neglected.

If the electron mobility ratio \( b \) differs from unity, then the magnitude of Hall coefficient will decrease as the square of the magnetic field increases. The relative change in \( R(B) \) could be expressed by

\[ \frac{\Delta R}{R_0 B^2} = \frac{R(B) - R_0}{R_0 B^2} \]  

(5-104)

\[ = -\frac{(n_1 + n_2)^2 \mu_1 n_1 n_2 (w - 1)^2}{(n_1 w + n_2)^2 (n_1 w^2 + n_2)} \]

Let \( p = \frac{n_1}{n_2} \), then

\[ \frac{\Delta R}{R_0 B^2} = -\frac{p (1 + p) (w - 1)^2 \mu_1^2}{(pw + 1)^2 (pw^2 + 1)} \]  

(5-105)

The Hall mobility \( \mu_H \) of this material could also be expressed as a function of \( w \) and \( p \) by

\[ \mu_H = R_0 \sigma_0 = R_0 (-e) (n_1 \mu_1 + n_2 \mu_2) \]  

(5-106)
The quantity $Q$ could be determined experimentally. And assuming $\mu_1$ is known, then the quantity $M$ could also be determined. In this case Equation (5-108) and (5-109) have two unknowns $w$ and $p$ which could easily be determined.

From Equation (5-109), it is seen that

$$ p = \frac{1 - Mw}{w^2(M - 1)} = \frac{Mw - 1}{w^2(1 - M)} \quad (5-110) $$

This could be used in Equation (5-108) to yield

$$ Q = - \frac{(1 - Mw)[1 + w - Mw]}{w^2M^3} (M - 1) $$
From this equation the solution for \( w \) is:

\[
w = \frac{(2M - 1)(M - 1)}{2M \left( (M - 1)^2 + QM^2 \right)} \]

\[
+ \frac{\left\{(M - 1)^2 - 4M^3 (M - 1)Q\right\}^{1/2}}{2M \left( (M - 1)^2 + QM^2 \right)}
\]

(5-111)

= the ratio of electronic mobilities \( \frac{\mu_1}{\mu_2} \).

The ratio of electron densities \( p \) could be obtained from Equation (5-110).

Now, with the help of the conductivity as measured in a small magnetic field, it is possible to determine \( n_1 \) and \( n_2 \)

\[
\sigma_o = -e (n_1\mu_1 + n_2\mu_2)
\]

\[
= e(n_1|\mu_1| + n_2|\mu_2|)
\]

\[
= e|\mu_1| n_1(1 + \frac{1}{pw})
\]

\[
\text{then } \quad n_1 = \frac{\sigma_o}{e|\mu_1| (1 + \frac{1}{pw})}
\]

(5-112)

and

\[
n_2 = \frac{n_1}{p} = \frac{\sigma_o}{e|\mu_1| [p + \frac{1}{w}]}
\]

(5-113)

Another Method to be used for materials where the ratio of electronic mobility is close to unity will be discussed in the remainder of this section.
In the previous method a measurement of \( \frac{\Delta R}{R_0 B^2} \) was necessary to determine \( p \) and \( w \) with the help of Hall mobility. For some materials of 2 kinds of charge carriers, the electronic mobilities may be comparable and the ratio \( w \) would be close to unity. In this case, it will be difficult to measure \( \frac{\Delta R}{R_0 B^2} \) as it will require a relatively higher magnetic field to produce enough change in the Hall coefficient beyond the error limits of the measuring apparatus.

For this reason, another method could be used. In this method, we deal with the change in \( R_0 \), the Hall coefficient in the limit of zero magnetic field, as the temperature is raised up to room temperature. This method was used\(^{35}\) by Iglitsyn and Yurova to evaluate the ratio \( p \) of the electron densities in a sample of GaAs\(_{0.6}\)P\(_{0.4}\).

The temperature dependence of the Hall coefficient and the Hall mobility is needed for this method.

At any temperature,

\[
R_0 = -\frac{1}{e} \frac{n_1w^2 + n_2}{(n_1w + n_2)^2}
\]

Let \( R' = -\frac{1}{e(n_1 + n_2)} = R_0 \bigg|_{w = 1} \)

And write \( R_0 \) as a Taylor series around \( w = 1 \) and keep two terms only, then

\[
R_0 = -\frac{1}{e(n_1 + n_2)} - \frac{n_1n_2}{e(n_1 + n_2)^3} (w - 1)^2,
\]

\[
= R' + R' \frac{n_1n_2}{(n_1 + n_2)^2} (w - 1)^2
\]
Then \[
\frac{R_0 - R'}{R'} = \frac{n_1n_2 (w - l)^2}{(n_1 + n_2)} \quad (5-116)
\]

Let \[
Y = \frac{R_0 - R'}{R'} = \frac{p (w - l)^2}{(1 + p)^2} \quad (5-117)
\]

At low temperature, the total number of electrons will be occupying the band of lower edge. And as the temperature increases the higher band will have an increasing number of electrons and the zero field Hall coefficient \(R_0\) will increase. By extrapolating the low temperature part of the curve up to room temperature we can get a reasonable value for \(R'\) which is the value of Hall coefficient at room temperature if there were no electrons being energized to the higher band.

Once more, the other equation relating \(p\) and \(w\) is Equation (5-109) for Hall mobility, written again here

\[
\frac{\mu_H}{\mu_1} = M = \frac{w^2p + 1}{w (wp + 1)} \quad (5-118)
\]

where the mobility \(\mu_1\) could be determined experimentally from a sample having electrons mainly in the (000) energy minima and the energy separation between the (000) edge and the \(<100>\) edges is \(\Delta E >> kT\).

Another way to get \(\mu_1\) is to extrapolate the temperature dependence of the mobility to room temperature. For GaAs\(_{1-x}\)Ga\(_x\), \(\mu_1\) is much larger than \(\mu_2\) and it is expected that \(\mu_H\), which is given by Equation (5-107) will have

\[
\mu_2 < \mu_H < \mu_1 \quad (5-119)
\]

From Equations (5-117) and (5-118), the solution for \(p\) and \(w\) could be obtained.
CHAPTER VI

SCATTERING MECHANISMS IN GaAs, P

6.1 Validity of the Relaxation Time Concept

The relaxation time $\tau$ determines the nature of the collision term $\left(\frac{\partial f}{\partial \tau}\right)_{\text{coll}}$ in Boltzmann's transport equation.

The relaxation time assumption is

$$
\left(\frac{\partial f}{\partial \tau}\right)_{\text{coll}} = \frac{f(K) - f_{0}(K)}{\tau(K)},
$$

(6-1)

where $f(K) - f_{0}(K)$ is the change added to the original equilibrium distribution function $f_{0}(K)$ due to the action of the perturbing forces.

The use of the relaxation time as a scalar quantity is justified only if the scattering is isotropic i.e., with equal probability along any direction. This is the case for spherical energy surfaces. GaAs was shown to have spherical energy valley at (000).

The transport equation approach, using a relaxation time, will be valid if the following conditions are satisfied:

First: the concept of a mean free path is meaningful, i.e.,

the duration of the collision $\Delta t$ is small compared to the time between two consecutive collisions $\tau$.  

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\[ \tau > \Delta t . \quad (6-2) \]

Second: The scattering is essentially elastic, i.e., if the change \( \Delta E \) of the carrier energy during collision is small compared to its energy \( E \),

\[ E > \Delta E . \quad (6-3) \]

But the Heisenberg uncertainty principle implies that

\[ \Delta E \Delta t = \hbar . \quad (6-4) \]

Then

\[ \tau E > \Delta E \Delta t = \hbar , \]

or

\[ \tau > \frac{\hbar}{E} . \quad (6-5) \]

6.2 Relaxation Times of Different Scattering Mechanisms.

The expressions for the relaxation times of the most important scattering mechanisms will be presented here together with the limits and conditions of their use. For each mechanism \( \tau \) could be written as \( \tau = \tau_0 x^r \), where \( x = \frac{E-E_C}{kT} \) for n-type semiconductor and the exponent \( r \) depends on the type of scattering.

6.2.1 Acoustical Phonon Scattering

This is the scattering by the longitudinal acoustical vibrations of the lattice. When an acoustical phonon is absorbed or emitted, the value of \( \Delta E \) is very small compared to \( E \); hence the
scattering is essentially elastic. For this scattering, the relaxation time is \(25, 29, 32\)

\[
\tau_L = \tau_0 L \times \frac{1}{x^2} 
\]  
(6-6)

\[
\tau_0 = \frac{2 \hbar^4 \rho u L^2}{\sqrt{2} E_1 (m^* kT)^{3/2}} 
\]  
(6-7)

where \(u_L\) = velocity of longitudinal sound waves

\(E_1\) = the change in band edge per unit dilation

\[
E_1 = \Omega \frac{dE_o}{d\Omega}
\]

\(E_o\) = energy of allowed band edge.

\(\Omega_o\) = initial volume of unit cell before deformation.

\(\rho\) = density of the semiconductor.

\(m^*\) = density-of-states effective mass.

This expression for the relaxation time is valid for temperatures \(T \gg 1^\circ K\) for semiconductors of all practically realizable carrier densities. \(25\) However, in principle, the value of \(\tau_L\) is not independent of the degree of doping of the semiconductor. The dependence of \(E_1\) on the doping level is not known since the lattice parameter may change with the impurity concentration. \(25\)

For the conduction band, the conductivity mobility is defined by \(\mu_c = -\frac{e}{m^*} <\tau>\). Then
\[ \mu_C = -\frac{e}{m_g} \tau_0 \langle x - \frac{1}{2} \rangle \] 

(6-8)

for acoustical phonon scattering, where \( m_g \) is the conductivity effective mass given for ellipsoidal energy surfaces by:

\[ \frac{1}{m_g} = \frac{1}{3} \left( \frac{1}{m_1} + \frac{1}{m_2} + \frac{1}{m_3} \right) \]

If Maxwell-Boltzmann statistics are used, then

\[ f_0(E) = e^{-\frac{E}{kT}} \]

(6-9)

And Equation (4-63) gives

\[ <x^r> = <\left(\frac{E-E_C}{kT}\right)^r> \]

(6-10)

\[
\begin{align*}
\int_{E_C}^{\infty} x^r E^{3/2} \frac{3f_0}{dE} \, dE &= \frac{\Gamma \left( r + \frac{5}{2} \right)}{\Gamma \left( \frac{5}{2} \right)} 
\end{align*}
\]

(6-11)

where \( \Gamma(s) \) is the gamma function defined by
\[
\Gamma(s) = \int_0^\infty t^{s-1} e^{-t} \, dt.
\]

For \( n = \) positive integer \( \geq 1 \), the gamma function will have

\[
\Gamma(n) = (n-1) \Gamma(n-1) = (n-1)!
\]

\[
\Gamma(1) = 0! = 1 \quad \text{and} \quad \Gamma\left(\frac{1}{2}\right) = \sqrt\pi.
\]

For acoustical phonon scattering, the conductivity mobility will be

\[
\mu_L = -\frac{4}{3\sqrt{\pi}} \frac{e}{m_0} \tau_0 \sim \frac{m_0^{-1}}{m_{\sigma}} \frac{m^*_{\sigma}^{-3/2}}{T^{-3/2}} \quad \text{(6-13)}
\]

And for spheroidal energy surfaces, the Hall mobility could be obtained, using Table (4-1), from its definition

\[
\mu_H \equiv \frac{R_0}{\rho_0} = -\frac{e}{m} \frac{<\tau^2>}{<\tau>} \frac{3K(2+K)}{(1+2K)^2} \quad \text{(6-14)}
\]

\[
= -\frac{e}{m_0} \tau_0 \frac{3\sqrt{\pi}}{2} \frac{3K(2+K)}{(1+2K)^2}
\]

Then

\[
\mu_H \sim \frac{m_0^{-1}}{m_{\sigma}} \frac{m^*_{\sigma}^{-3/2}}{T^{-3/2}}. \quad \text{(6-15)}
\]

And for acoustical phonon scattering and spheroidal energy surfaces, the Hall coefficient factor \( r \) will be

\[
r = \frac{\mu_H}{\mu_L} = \frac{3\pi}{8} \frac{3K(2+K)}{(1+2K)^2} \quad \text{(6-16)}
\]
One clearly see that for acoustical phonon scattering, the mobility has $T^{-3/2}$ temperature dependence.

The transverse magnetoresistance expression for this scattering in an isotropic medium is

$$\frac{\Delta \rho}{\rho_0 B^2} = \frac{e^2}{m^* 2} \left[ \frac{\langle \tau^3 \rangle}{\langle \tau \rangle} - \frac{\langle \tau^2 \rangle}{\langle \tau \rangle^2} \right]$$

Then

$$\frac{\Delta \rho}{\rho_0 B^2} = \frac{e^2}{m^* 2} \frac{2}{\tau_0 L} \left( 1 - \frac{\pi}{4} \right)$$

$$\sim (m^*)^{-5} T^{-3} \quad (6-17)$$

Therefore, for small magnetic fields and acoustical phonon scattering, the transverse magnetoresistance varies as $T^{-3}$ with the temperature.

In III-V compounds, scattering by acoustical phonons is important in limiting the mobility as long as the average thermal energy $kT$ is small compared to the energy of the optical phonons and provided that any impurity or intervalley scattering is small.

6.2.2 Optical Phonon Scattering

This type of scattering, in crystal structures of more than one atom in the unit cell, is due to the interactions between charge carriers and the optical vibrations of the lattice atoms. In this optical phonon scattering $\Delta E$, which is equal to $\pm \hbar \omega$, may be larger or
smaller than the energy of the charge carrier depending on the temperature. At high temperatures when $\hbar \omega_o \ll kT$ the optical phonon scattering could be regarded as elastic. At low temperatures when $\hbar \omega_o \gg kT$, the optical phonons absorbed by the electrons greatly changes their energy. Consequently, the concept of relaxation time loses its meaning. However, if we neglect the time during which the electron is in a high energy state, we can still use the relaxation time concept.\textsuperscript{25}

In this case the relaxation time was shown\textsuperscript{25} to be:

$$\tau = \tau_0 \quad , \quad x = 0 \quad \text{in expression (6-18)}$$

$$\tau = \tau_0 x^r$$

For heavily doped semiconductors $\frac{\xi}{kT} > 0$, and at $T \ll \theta_D$ the Debye temperature

$$\tau = \tau_0 = \frac{a^3 M}{2\pi \sqrt{2m^*}} \frac{(h\omega_o)^{3/2}}{(\gamma ze^2)^2} \frac{\exp \left( \frac{h\omega_o}{kT} \right)}{\left( 1 - f_o \right)}$$

And for lightly doped semiconductors $\frac{\xi}{kT} < 0$ and at $T \ll \theta_D$

$$\tau = \tau_0 = \frac{a^3 M}{2\pi \sqrt{2m^*}} \frac{(h\omega_o)^{3/2}}{(\gamma ze^2)^2} \frac{\exp \left( \frac{h\omega_o}{kT} \right)}{\left( 1 - f_o \right)}$$

And at higher temperatures $T \gg \theta_D$

$$\tau_0 = \frac{a^3 M}{2\pi \sqrt{2m^*}kT} \left[ \frac{h\omega_o}{\gamma ze^2} \right]^2$$

for any degree of doping.
In these expressions, the notations used are:

\[ a = \text{lattice parameter} \]
\[ \omega_o = \text{limiting frequency of longitudinal optical vibrations} \]
\[ M = \text{atomic mass} \]
\[ Ze = \text{ionic charge} \]
\[ \gamma = \text{polarization factor of ions} \]

6.2.3. Scattering by Ionized Impurities

An ionized impurity center in the lattice of a semiconductor produces a long-range Coulomb field of potential \( \frac{e}{K_d s} \) at a distance \( s \), where \( K_d \) is the dielectric constant.

Brooks and Herring allowed for the fact that the free carriers may collect around a charged center and partly screen its potential. Expressing this screened potential as \( V(s) = \left( \frac{e}{K_d s} \right) e^{-F_0} \). The screening radius \( R_s \) for any degree of degeneracy is given by

\[
\frac{1}{R_s^2} = \frac{16 \pi^2 e^2 (m^*)^{3/2}}{h^3 K_d} \frac{1}{(2kT)^{1/2}} \quad F_0 = \frac{\zeta}{(kT)}
\]

In the absence of degeneracy, \( R_s \) reduces to

\[
R_s = \frac{K_d}{(kT)} \frac{1/2}{2\sqrt{\pi} e\sqrt{n^*}}
\]

where \( n^* \) depends on the degree of compensation, and is given by
\[ n^* = n + (n + N_d) \left[ 1 - \frac{n + N_a}{N_d} \right], \]

for n-type semiconductor of donor concentration \( N_d \), acceptor concentration \( N_a \) and electron concentration \( n \). For slight compensation \( n^* = n \).

In this type of scattering, the relaxation time is given by

\[ \tau_i = \tau_{i0} x^{3/2}, \quad \text{where} \quad x = \frac{E-E_C}{kT} \quad (6-19) \]

\[ \tau_{i0} = \frac{\sqrt{2\pi m K_d}}{n e N_i g}, \quad (6-20) \]

\( N_i \equiv \text{total number of ionized impurities, both donor and acceptors,} \]

\[ g = \ln (1+b) - \frac{b}{1+b}, \]

and

\[ b = \frac{2m*K_{ix}(kT)^2}{n e^2 n^2 h^2} \]

For ionized impurity scattering, low magnetic field and spherical band structure, the mobility is\(^{29}\)

\[ \mu_i \sim \frac{3/2}{(kT) K_d^{2}} \frac{\sqrt{m^* N_i g}}{N_i} \quad (6-21) \]

for any degree of degeneracy, and the magnetoresistance for this case has\(^{29}\)

\[ \frac{\Delta \rho}{\rho_0 B^2} \sim \frac{\tau_{i0}}{m^* g^2} \sim \frac{K_d}{m N_i g^4} \quad (6-22) \]

at low magnetic field.
6.2.4. Scattering by Neutral Impurities

This scattering mechanism is unimportant except for lightly doped semiconductors at sufficiently low temperatures. The relaxation time is given by

\[ \tau_N = \frac{(m^*)^2 e^2}{20 h^3 k_B N_d N_n} \]

6.2.5. Polar Optical Scattering

GaAs\(_{1-x}\)P\(_x\), and other III-V compounds and alloys, can support optical as well as acoustical vibrational modes. The atoms in a unit cell have different resultant electric charges which give these semiconductors their partly ionic character. The electrostatic interaction between the charge carriers and the internal polarization field due to optical vibrations is one of the most important scattering mechanisms in the III-V compounds and their alloys.

In the diamond structure, the two atoms of the unit cell are the same and the associated nonpolar optical interaction is of only minor importance relative to the acoustical phonon interaction or to the ionized impurities interaction.

For III-V semiconductors of small electron effective mass the polar interaction is much stronger than the deformation potential interaction. However, for the multivalley conduction band of GaAs\(_{1-x}\)P\(_x\), the \(<100>\) valleys deformation potential may be comparable to the polar optical scattering.
No relaxation time can be defined\textsuperscript{6} for polar optical scattering. The transport coefficients can no longer be expressed as integrals over various powers of the relaxation time and energy.

Ehrenreich\textsuperscript{18} showed that for n-type GaAs, the polar optical scattering is the dominant one above room temperature and when reasonably large concentrations of electrons are present the polar interaction is screened. For the case of combined polar optical scattering and scattering by ionized impurities, Ehrenrich calculated the mobility taking into account the screening effects and neglecting the \textlangle 100\textrangle valleys of GaAs conduction band. This expression for the mobility is\textsuperscript{6}

\[
\mu = \left(\frac{2}{3}\pi e^{*} m^{*} \right)^{1/2} \frac{1}{e} \frac{\hbar \omega_{\text{L}}}{kT} \left[ e \frac{\hbar \omega_{\text{L}}}{kT} - 1 \right] \frac{G_{1}\left(\frac{\zeta}{kT}, \frac{\hbar \omega_{\text{L}}}{kT} \right)}{F_{1/2}\left(\frac{\zeta}{kT} \right)}
\]  

(6-23)

where \( M \equiv \) the reduced mass of the two different atoms in GaAs

\( v_{a} \equiv \) volume of unit cell

\( \omega_{\text{L}} \equiv \) optical frequency of longitudinal lattice vibrations

\( e^{*} \equiv \) effective ionic charge.

The function \( G_{1} \) contains the effect of the combined scattering mechanisms, degeneracy and the departure of band structure from isotropic parabolic behavior.
CHAPTER VII
EXPERIMENTAL PROCEDURE

7.1 Sample Preparation

Wafers of epitaxially deposited GaAs$_{1-x}$P$_x$ were kindly supplied by Monsanto Company. The epitaxial layer, doped with tellurium impurity, was deposited on (100) GaAs substrates of much lower resistivity with the phosphorus mole fraction $x$ gradually increasing in a transition region at an approximate rate of 0.01 phosphorus mole fraction in one micron.

In addition to the samples made from this epitaxially deposited GaAs$_{1-x}$P$_x$, additional samples were made from (111) wafers of GaAs:Ge-doped, GaAs:Te-doped and GaP.

The samples were fabricated in a bridge shape with six potential arms as shown in Plate I. The steps necessarily taken to prepare these samples from the wafers will be described subsequently in this section.

7.1.1 Sample Orientation

Before cutting each sample, the wafer orientation was checked and the direction of sample length was chosen using the light figures orientation method. In this method a characteristic light figure is reflected from a lapped surface illuminated by a narrow light beam. The technique is based on the fact that in Ge, Si and III-V semiconductors the majority of the facets in a lapped surface have (110)
Plate I. Sample placed on its holder and with the leads connected (enlarged 5 X).
Figure (7-1). Shape and dimensions of samples used. They were ultrasonically cut by a tool of slightly larger dimensions. All dimensions shown here are in inches.
orientations, thus reflecting light in a way characteristic of the orientation of that lapped surface.

Orientation was made here using the wafer back surface. This surface was lapped on a glass plate by Aluminum Oxide abrasive of grit size 240, then rinsed in distilled water and dried. A light beam passing through a pinhole in a screen is reflected from this lapped surface, and light figures appear on the screen. The wafer was waxed to a microscope slide and its position repeatedly adjusted by heating the wax until the chosen direction of the sample length was parallel to a known direction in the glass slide.

7.1.2 Ultrasonic Cutting of Bridge Shaped Samples

After choosing the direction of sample length and with the sample waxed to the microscope slide, the assembly is transferred to an ultrasonic cutting machine. The ultrasonic cutting tool and cone are shown in Plate II.

The tool was made of two stainless steel pieces tightly held together. This allowed the use of 10 mil slicing wheels to cut the grooves of the sample potential arms while the two pieces are held side by side. Three slicing operations were enough to cut the six 10 mil grooves. Then the two pieces were accurately held in position and brazed together at 950°C in a dry hydrogen atmosphere using a nickel-gold alloy. After that, the tool was brazed to the cone by R.F. heating using silver-copper eutectic in a stream of forming gas. The cutting surface of the tool was regularly ground flat after cutting four or five samples.
Plate II. Ultrasonic cutting tool and cone (enlarged 2 X).
Raytheon ultrasonic generator and transducer [Impact Grinder Model 2-334] were used in this process. The abrasive used was boron carbide of grain size 800 and the vertically applied force was about 12 ounces. With the back surface waxed to the microscope slide, the sample was cut to the desired thickness and then removed and lapped by a lapping compound of grain size 1800 from the back surface. With this arrangement the potential arms of the sample did not get broken. Many samples were damaged before using this procedure when the ultrasonic cutting was made all the way through the total thickness.

Figure (7-1) shows a bridge shaped sample and its dimensions.

7.1.3 Sample Contacting

After ultrasonically cutting the sample and lapping the back surface to remove the GaAs substrate and the transition layer where the phosphorus content is not uniform, contacts were made using a strip heater and forming gas atmosphere (10% H₂, 90% N₂). The sample was first degreased by acetone or methanol and then etched in 50 ml of 3 HSO₄: 1 H₂O₂ : 1 H₂O for about 30 seconds with continuous stirring of the etchant. After that it was rinsed thoroughly with distilled water by decantation, i.e., without exposing the sample to the air until it was completely rinsed of the etchant. The sample was then dried and placed in the strip heater. With little clean chips of the contact material placed on the sample and with the strip heater cover on, it was left for about 5 minutes with forming gas flowing. Current was
then gradually passed through the strip heater until the little chips melted into bright semispheres. The current was then turned off and the sample left to cool for about 10 minutes in a stream of forming gas.

The contacts made this way were ohmic and of low resistance. The same method was used for all the samples. With each sample having eight contacts of differing areas, the I-V characteristics were found to be ohmic between any two contacts. This indicates that each contact is ohmic. Ohmic contacts are necessary when making transport measurements to avoid contributions of rectifying barriers to the measured voltages.

The contacting material, used for the n-type nondegenerate samples of this research, was an alloy of 75% In, 16% Pb, 5% Ag, 2% Te and 2% Sn.

7.1.4 Sample Holder and Encapsulation

The sample was pasted by thermal grease on a quartz plate which in turn was pasted on a copper disc. Leads made of vinyl insulated stranded wire pass through holes in this copper disc and in each wire all the strands were cut except one which was soldered to the sample contact with a small clean soldering tip and without using any flux. This arrangement is shown in Plate (I).

An Amphenol 9 pin cable connector type (126-220) was modified and used to carry the sample holder in two configurations as shown in Plate III and Plate IV. To avoid the risk of breaking the samples, each sample was mounted in a plug and enclosed by a pyrex glass capsule.
Plate III. Sample placed in the first configuration; where the magnetic field is directed horizontally and is always perpendicular to sample width. The angle controlling mechanism is also shown here.
Plate IV. A sample and its holder placed in the second configuration; where the sample large surfaces are parallel to the magnetic field. The pyrex glass capsule is not shown here.
made from the end of a 17 mm O.D. test tube. The assembly of the pyrex capsule and the plug was then sealed by a few turns of a scotch adhesive tape.

Encapsulation in this way proved to be essential for two purposes. The first purpose is to keep the sample from being broken when suddenly cooled by liquid nitrogen. Many samples were thermally shocked and cracked when quickly cooled by liquid nitrogen without this encapsulation. The second purpose is to reduce the thermal fluctuations which greatly affect the resistivity and Hall effect measurements.

When taking data at liquid nitrogen temperatures, the encapsulated sample would reach this temperature in about 25 minutes after dipping its assembly in the liquid nitrogen. During that time the leakage through the scotch tape would be enough to equalize the pressure in and out of the capsule and to introduce liquid nitrogen around the sample. When heating back to room temperature, this leakage proved useful in releasing the evaporating nitrogen inside the capsule.

This arrangement for holding the sample and encapsulating it proved to be successful from room temperature down to 4°K.

7.2 Measuring Apparatus

The apparatus used for measuring the galvanomagnetic properties of these samples consists of:

1. Constant Current Source
Figure (7-2). Schematic Diagram for the Measuring Apparatus.
3. Varian Associates regulated magnet
4. Gaussmeter
5. Terminal and Switching Board
6. Digital Voltmeter

A schematic block diagram is shown in Figure (7-2). The constant current source was made of a regulated voltage power supply (Model 1545, Power Design, Inc.) with 2.5 MΩ, 2.5 Watt resistor in series with the sample. A digital voltmeter was used to measure the sample current by measuring the voltage across a 100 ohm 0.05% resistor in the sample circuit. The fluctuations in the current were kept below 0.02% by adjusting the series resistors and the regulated voltage supply.

For liquid nitrogen measurements, the liquid nitrogen dewar was loosely covered to reduce the convective thermal currents at the air and liquid nitrogen interface which disturbs the measurements.

Some measurements were made by using a variable temperature dewar [Janis Research Company, Model DT] to vary the temperature from 4°K to 300°K.

Plates V, VI, VII show the arrangements for taking the measurements at room temperature, liquid nitrogen temperature and at variable temperatures, respectively.

In Plate VII, the panel on the left side contains the temperature controller, the dewar jacket vacuum gauge and the valves, pressure regulator and pressure gauges necessary to adjust the flow
Plate V. Arrangement for making measurements at room temperature.
Plate VI. Arrangements for making measurements at liquid nitrogen temperature.
Plate VII. Arrangement for making measurements at variable temperature; from 4°K to 300°K.
of helium gas to the helium path and/or to the sample chamber. In the
controlled temperature dewar, the sample temperature was that of a
steady flow of He gas whose temperature was controlled by the tempera-
ture controller using 1/2 amp., 5 watt heater and a gallium arsenide
diode as a sensor. Another GaAs diode was used to measure the tempera-
ture at the sample.
CHAPTER VIII
RESULTS AND DISCUSSION

In this chapter, the experimental data will be presented and related to the theoretical analysis presented thus far. Samples were prepared as described in the preceding chapter.

It was of special interest in this research to study the conductivity, Hall coefficient and magnetoresistance of the two conduction bands in the GaAs$_{1-x}$P$_x$. The presence of two kinds of carriers, belonging to two conduction bands in this semiconductor alloy, are most noticeable for $x < 0.44$ or $0.45$. When $x$ is larger, the effect is smaller due to the larger density of states associated with the $<100>$ valleys which reduces the chance of getting electrons energized to the (000) low effective mass valley.

Not all the samples survived the testing at all temperatures. The differential expansions and contractions between the first samples and their holders were responsible for breaking some of them. Also some samples were lost due to thermal shock when quickly cooled by liquid nitrogen. To reduce the thermal shocking effects, a special pyrex glass capsule was used to contain the sample. This and other precautions are described in the experimental procedure chapter.

The samples used are listed in Table (8-1) together with their properties at room and liquid nitrogen temperatures. All the
<table>
<thead>
<tr>
<th>Sample</th>
<th>Phosphorus Mole Fraction</th>
<th>Wafer Surface Orientation</th>
<th>Sample Length Direction</th>
<th>Sample Thickness in mils</th>
<th>Data at 297°K</th>
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</thead>
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<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>$P_o$ cm</td>
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<td>23 GaAs:Ge-doped</td>
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<td>(111)</td>
<td>[112]</td>
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<td>0</td>
<td>(111)</td>
<td>[112]</td>
<td>15.8</td>
<td>0.0267</td>
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<td>16 GaAs$<em>{0.86}$P$</em>{0.14}$</td>
<td>0.14</td>
<td>(100)</td>
<td>[110]</td>
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<td>0.0013</td>
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<tr>
<td>17 GaAs$<em>{0.86}$P$</em>{0.14}$</td>
<td>0.14</td>
<td>(100)</td>
<td>[100]</td>
<td>5.5</td>
<td>0.0013</td>
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<tr>
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<td>0.288</td>
<td>(100)</td>
<td>[110]</td>
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<td>(100)</td>
<td>[110]</td>
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<td>0.175</td>
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<td>(100)</td>
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</tr>
<tr>
<td>18 GaAs$<em>{0.60}$P$</em>{0.40}$</td>
<td>0.40</td>
<td>(100)</td>
<td>[110]</td>
<td>4.8</td>
<td>0.5362</td>
</tr>
<tr>
<td>19 GaAs$<em>{0.60}$P$</em>{0.40}$</td>
<td>0.40</td>
<td>(100)</td>
<td>[100]</td>
<td>4.8</td>
<td>0.485</td>
</tr>
<tr>
<td>30 GaAs$<em>{0.5686}$P$</em>{0.4314}$</td>
<td>0.4314</td>
<td>(100)</td>
<td>[110]</td>
<td>5.5</td>
<td>3.553</td>
</tr>
<tr>
<td>33 GaAs$<em>{0.5686}$P$</em>{0.4314}$</td>
<td>0.4314</td>
<td>(100)</td>
<td>[110]</td>
<td>5.0</td>
<td>2.1687</td>
</tr>
<tr>
<td>34 GaAs$<em>{0.5087}$P$</em>{0.4913}$</td>
<td>0.4913</td>
<td>(100)</td>
<td>[110]</td>
<td>5.1</td>
<td>4.7226</td>
</tr>
<tr>
<td>32 GaAs$<em>{0.4993}$P$</em>{0.5007}$</td>
<td>0.5007</td>
<td>(100)</td>
<td>[110]</td>
<td>6.5</td>
<td>0.676</td>
</tr>
<tr>
<td>29 GaP</td>
<td>1.00</td>
<td>(111)</td>
<td>[112]</td>
<td>20.0</td>
<td>0.0218</td>
</tr>
</tbody>
</table>
samples listed in this table, except the upper two and the first one, are made from wafers of epitaxially deposited GaAs$_{1-x}$P$_x$ with tellurium impurities on GaAs substrates.

At room temperature, a uniform magnetic field up to 19 Kilogauss was applied to each sample to determine the magnetoresistance $\frac{\Delta \rho}{\rho_0}$ and the Hall coefficient $R(B)$. To get the same data at 77°K, the magnet air gap was increased to allow for a liquid nitrogen dewar. This limited the magnetic field to 12 Kilogauss.

Unless otherwise indicated, the dependence of magnetoresistance $\frac{\Delta \rho}{\rho_0}$ on the magnetic field was measured with the sample placed in the first configuration and transverse to the magnetic field.

The electron density ratio $\frac{n_2}{n_1}$ is essential in this discussion for ascertaining the relative importance of the low and the high mobility electrons. This ratio will be estimated for nondegenerate conditions by using the following equations which were discussed in Chapters II and III:

\[ m^* = 0.072 \ (1 + x) \ m_o \]  
\[ m^*_2 = 1.2 \ m_o = \text{density-of-states effective mass of } \langle 100 \rangle \text{ conduction band spheroids} \]  
\[ \frac{n_2}{n_1} = \left[ \frac{m^*_2}{m^*_1} \right]^{3/2} e^{-\frac{\Delta E}{kT}} \]  
\[ \Delta E = E_2 - E_1 \]

At 295°K, $\Delta E = 0.35 - 0.69 x - 0.2 x^2$.  (8-5)

At 77°K, $\Delta E = 0.37 - 0.71 x - 0.2 x^2$.  (8-6)

The ratio $\frac{n_2}{n_1}$ is shown in Figure (8-1) as a function of the
Figure (8-1). Variation of $\frac{n_2}{n_1}$ with $x$ for GaAs$_{1-x}$P$_x$ at 297°K and 77°K.
phosphorus mole fraction $x$ at room temperature and at liquid nitrogen temperature.

8.1 Magnetoresistance $\frac{\Delta \rho}{\rho_0}$

For small magnetic fields, the magnetoresistance was found to increase linearly with $B^2$ for all samples at room temperature. As the magnetic field increases, and the small field condition, $\mu B \ll 1$, is no longer valid, $\frac{\Delta \rho}{\rho_0}$ deviates from this $B^2$ dependence. This could be seen for samples (23 GaAs:Ge-doped) and (24 GaAs:Te-doped) in Figures (8-2a) and (8-3), respectively. Also, such behavior was recorded for sample 10 GaAs$_{0.65}$P$_{0.349}$ at 297°K as shown in Figure (8-6a). Due to the lower mobility of the other samples, no deviation of $B^2$ dependence was detected within the available range of the magnetic field density.

At 77°K, and for small magnetic fields, $\frac{\Delta \rho}{\rho_0}$ was found to be linearly proportional to $B^2$ also, although for some samples a negative magnetoresistance was recorded possibly due to inhomogeneity of charge carrier distribution.

The heavily doped sample 16 GaAs$_{0.86}P_{0.14}$ shows essentially the same properties at room temperature and at 77°K. $\frac{\Delta \rho}{\rho_0}$ was found zero for this sample at both temperatures where $n_1 >> n_2$ and there are essentially no contribution from the electrons in the $<100>$ valleys. The vanishing transverse magnetoresistance for this sample indicates that $b = 0$, where

$$b = \frac{\rho_{1122}}{\rho_0} = \frac{e^2}{m^2} \left[ \frac{\langle \tau_1^3 \rangle}{\langle \tau_1 \rangle} - \frac{\langle \tau_1^2 \rangle^2}{\langle \tau_1 \rangle^2} \right]. \quad (8-7)$$
Figure (8-2). $\frac{\Delta \rho}{\rho_o}$ % for sample 23 GaAs:Ge-doped, (a) Transverse $\frac{\Delta \rho}{\rho_o}$ %, (b) Angular Variation.
Figure (8-3). Transverse $\frac{\Delta \rho}{\rho_0}$ % for sample 24 GaAs:Te-doped.
This was expected since the relaxation time is essentially independent of the energy for heavily doped semiconductors.

Figure (8-4) shows the variation of $\frac{\Delta \rho}{\rho_0}$ with the magnetic field for the sample 14 GaAs$_{0.712}P_{0.288}$ at three different temperatures. At 4.2°K, the magnetoresistance was negative and proportional to $-B^{0.6}$ as deduced from plotting it on a log-log graph paper. The reasons for the negative magnetoresistance at this temperature are not clearly understood.

The angular variation of $\frac{\Delta \rho}{\rho_0}$ was recorded for some samples. The longitudinal magnetoresistance is expected to be zero for GaAs$_{1-x}$P$_x$ when $n_2$ is small enough and energy surfaces are spherical. For most of the samples where this condition is satisfied, the longitudinal magnetoresistance did not vanish. It is suspected that the inhomogeneity of charge carriers is responsible for this nonvanishing longitudinal magnetoresistance. 41

Figure (8-5) shows the angular variation of $\frac{\Delta \rho}{\rho_0}$ for the sample 14 GaAs$_{0.712}P_{0.288}$ at different temperatures and different magnetic fields. At 77°K, $\frac{\Delta \rho}{\rho_0}$ appears to have a positive part superimposed on a negative constant part. The positive part increased 4 times when the magnetic field was doubled. At 4.4°K, the magnetoresistance is negative and has no angular variation.

In making measurements of $\frac{\Delta \rho}{\rho_0}$ at different angles or at different magnetic fields, the temperature of the sample must be stable enough to preclude the masking of the true magnetoresistance change
Figure (8-4). Transverse $\frac{\Delta \rho}{\rho_o}$ for sample $14 \text{ GaAs}_{0.712}\text{P}_{0.288}$. 
Figure (8-5). Angular Variation of $\frac{\Delta \rho}{\rho_0}$ for sample 14 GaAs $P_{0.712 \theta 0.288}$. 

$\theta$ in degrees

$\frac{\Delta \rho}{\rho_0}$ %
Figure 8-6. $\frac{\Delta \rho}{\rho_0}$% for samples 11 GaAs$_{0.651}$P$_{0.349}$ and 10 GaAs$_{0.651}$P$_{0.349}$. 

(a) Transverse Magnetoresistance

(b) Angular Variation
by the spurious changes due to thermal fluctuations. In most of the measurements reported here, the values of $\frac{\Delta \rho}{\rho_0}$ are not the same at 0° and 180° mainly because of temperature fluctuations and drifts which were difficult to eliminate completely. For example as shown in Figure (8-5) for sample 14 GaAs $P_{0.712 0.288}$, a magnetic field larger than 10 K Gauss was necessary to unmask the angular variation of the bulk magnetoresistance from those effects due to thermal fluctuations and sample surface.

8.2 Seitz Magnetoresistance Coefficients

The Seitz magnetoresistance coefficients $b$, $c$ and $d$ were calculated for these samples using Equations (5-79) to (5-85). Table (8-2) shows the values of these coefficients for some samples at 297°K and 77°K. The data presented in this table are based on measurements shown in Figures (8-2) and (8-7) to (8-11).

It is clear from this table that for samples of $x = 0.0.40$ or more, $b \neq -c$ and $d < 0$. This suggests the existence of $<100>$ valleys in the conduction band of these alloys since from Equations (5-86) to (5-89), it is seen that $d$ is negative for the $<110>$ or $<110>$ valleys.

In evaluating Seitz magnetoresistance coefficients $b$, $c$ and $d$ it was found that using two samples does not give consistent results due to the difficulty of obtaining two exactly similar samples that differ only in the length direction. This was attempted by using samples 18 GaAs$_{0.6}P_{0.4}$ and 19 GaAs$_{0.6}P_{0.4}$ which have (100) surface orientation and their lengths are along [110] and [100] directions, respectively.
# Table (8-2)

## Seitz Magnetoresistance Coefficients for Some Samples

<table>
<thead>
<tr>
<th>Sample</th>
<th>Temperature</th>
<th>Experimental Results</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Units of b, c, d in cm$^4$/volt$^2$sec$^2$</td>
</tr>
</tbody>
</table>
| 23 GaAs: Ge-doped | 297$^\circ$K | b + c + 1/2 d = 52000  
                  |             | b + 1/2 c + 0.181 d = 253000  
                  |             | b + 1/3 d = 453000 | 454500 | -400300 | -4500 |
| 18 GaAs $0.60^P0.40$ | 297$^\circ$K | b + c + 1/2 d = 12.7 $\times$ 10$^6$, b = 144 $\times$ 10$^6$  
                  |             | b + c + d = 6.5 $\times$ 10$^6$, b = 131 $\times$ 10$^6$ | 140 $\times$ 10$^6$ | -121 $\times$ 10$^6$ | -12.4 $\times$ 10$^6$ |
| 19 GaAs $0.60^P0.40$ | 297$^\circ$K | From 1st configuration b = 1.860 $\times$ 10$^6$  
                  |             | From 2nd configuration b + 1/2 d = 1.81 $\times$ 10$^6$ | 1.86 $\times$ 10$^6$ | -10$^5$ |
| 33 GaAs $0.5686^P0.4314$ | 297$^\circ$K | From 1st configuration b = 11.56 $\times$ 10$^6$  
                  | 77$^\circ$K  | From 2nd configuration b + 1/2 d = 10.26 $\times$ 10$^6$ | 11.56 $\times$ 10$^6$ | -8.66 $\times$ 10$^6$ | -2.6 $\times$ 10$^6$ |
| 34 GaAs $0.5087^P0.4913$ | 297$^\circ$K | From transverse $\Delta \rho \over \rho_0$, b = 70000  
                  |             | From longitudinal $\Delta \rho \over \rho_0$, b + c + 1/2 d = 5700 | 70000 | -46400 | -35800 |
| 32 GaAs $0.4993^P0.5007$ | 297$^\circ$K | From 1st configuration $b = 40.7 \times 10^3$  
                  |             | From 2nd configuration:  
                  |             | $\Delta \rho \over \rho_0$ at $\theta = 90^\circ$ gives b + 1/2 d = 29.3 $\times$ 10$^3$ | 40700 | 29200 | -22800 |
Consistent results were obtained by using samples of (111) surfaces with [112] length direction, or by placing the samples of (001) surface and [110] length direction in two different configurations with respect to the magnetic field as indicated in Section 5.2. The longitudinal magnetoresistance for these two configurations should be the same due to the cubic symmetry. In practice this was not the case because of the inhomogeneity of charge carrier distribution. It is suspected that some voltages produced by this inhomogeneity contribute to the measured \( \frac{\Delta \rho}{\rho_0} \) when the sample is in the first configuration. This effect was largely reduced by placing the sample in the second configuration where the thin sample has its flat surfaces planar with the magnetic field.

8.3 Determination of the Effective Mass Anisotropy Ratio of <100> Valleys

The data obtained for sample 34 GaAs\(_{0.5087}\)P\(_{0.4913}\) could be used to determine the effective mass anisotropy ratio K of the <100> valleys, where K = \( \frac{m_1}{m_2} = \frac{m_1}{m_3} \) as shown by Equations (4-68) and (4-69). The value of K at room temperature could be obtained by incorporating the data given in Table (8-2) about this sample together with its Hall mobility into Equation (5-98) with the approximation \( \frac{n_1}{n_2} = 0 \). This approximation is justified since at 297°K, Equation (8-5) gives \( \Delta E = -0.037 \text{ eV} \) and the ratio \( \frac{n_1}{n_2} \), as given by Equations (8-1) to (8-4), could be written as

\[
\frac{n_1}{n_2} = \left( \frac{m^*}{m_{2d}} \right)^{3/2} \text{e}^{\frac{\Delta E}{q}} = \frac{1}{37.5} \text{e}^{-1.44} = \frac{1}{160}
\]
(a) Transverse Magnetoresistance

Figure (8-7). $\frac{\Delta \rho}{\rho_0} \%$ for samples 18 GaAs$_{0.60}$P$_{0.40}$ and 19 GaAs$_{0.60}$P$_{0.40}$. 

(b) Angular Variation

Samples placed in first configuration
Figure (8-8). $\frac{\Delta \rho}{\rho}$ for sample 30 GaAs$_{0.5586}$P$_{0.4314}$.
Figure (8-9). $\frac{\Delta \rho}{\rho_o} \%$ for sample 33 GaAs $P_0.4314$. 

(a) Transverse Magnetoresistance

(b) Angular Variation
Figure (8-10). \( \frac{\Delta \rho}{\rho_0} \) for sample 34 GaAs\(_{0.5087}P_{0.4913}\).
Figure (8-11). Angular variation of magnetoresistance for sample 32 GaAs$_{0.4993}$P$_{0.5007}$. 
Therefore, Equation (5-98) could be written as

\[
\frac{b + c + \frac{1}{2} d}{b + \frac{2}{H}} = \frac{(K - 1)^2}{2(1 + K + K^2)} \tag{8-8}
\]

Measurements made on this sample are shown in Figures (8-10a,b,c).

The following data were obtained:

\[
b + c + \frac{1}{2} d = 5,700 \text{ cm}^4/\text{volt}^2\text{sec}^2
\]

\[
b = 70,000 \text{ cm}^4/\text{volt}^2\text{sec}^2
\]

\[
\mu_H = 190 \text{ cm}^2/\text{volt sec}.
\]

This lead, after solving Equation (8-8) which is a second degree algebraic equation, to two values of \(K\); namely

\[
K = 1.81 \text{ or } K = 0.55
\]

These values are the reciprocals of each other as expected from Equation (8-8) when substituting \(\frac{1}{K}\) instead of \(K\).

The effective mass ratio \(K\) is known to be 20 for Germanium and to be 5 for silicon. This indicates prolate spheroidal energy surfaces. By comparison to the case of silicon, the effective mass ratio for GaAs \(P_{0.5087}^{0.4913}\) at room temperature is probably greater than unity and thus has the value \(K = 1.81\).

With such a small value for \(K\), the relaxation time anisotropy is not likely to be significant. This justifies ignoring the relaxation time anisotropy ratio in the analysis presented in Chapters IV, V and VI. Therefore, the relaxation time could be assumed isotropic especially at room temperature.
8.4 Determination of the Mobilities and Densities of the Electrons in the Different Conduction Bands

When the conduction bands at (000) and along <100> are simultaneously populated, one cannot get an exact determination of the electron mobility or density from the measurements of the Hall coefficient and the resistivity alone. The values derived from these parameters should only be used as rough estimations of the electron mobility and density.

The method presented in the beginning of Section 5.5 will be used here to illustrate this point and to give a better estimate of the electron densities and mobilities for sample 30 GaAs at room temperature.

The change in the Hall coefficient R(B) with the magnetic field at room temperature is shown in Figure (8-12) for this sample. From this change, it is possible to estimate the quantity Q defined in Equation (5-108). For $B = B_1$ Kilo gauss and $\mu_H$ in cm$^2$/volt sec.

$$Q = \frac{\Delta R}{R_0 B_1^2 \mu_H} = \frac{\Delta R}{R_0 B_1^2 \mu_H} 10^{10} = -0.391.$$

There are 3 unknowns in Equations (5-108) and (5-109), namely $w = \frac{\mu_1}{\mu_2}$, $p = \frac{n_1}{n_2}$, and $\mu_1$. In the analysis following these equations, $\mu_1$ was assumed to be known and the values of $w$ and $p$ are to be determined. For this sample, which has $x = 0.4314$, it is relatively safer to evaluate the ratio $p = \frac{n_1}{n_2}$ and to assume $\mu_1$ and $\frac{\mu_1}{\mu_2}$ as the two unknowns. The ratio $p$ could be obtained from Equation (3-30). This
Figure (8-12). Hall coefficient for sample 30 GaAs$_{0.5686}P_{0.4314}$. 

The graph shows the Hall coefficient ($R(B)\text{ Hall Coefficient cm}^3/\text{coulomb}$) as a function of temperature. The data points are plotted along a line that represents the equation $30\text{ GaAs}_{0.5686}P_{0.4314}$ at 297°K.
only requires knowledge of \( x \); the phosphorus mole fraction. For this sample at room temperature, the ratio \( \frac{n_2}{n_1} = 20 \) as obtained from Figure (8-1). Then \( p = \frac{n_1}{n_2} = 0.05 \) and Equation (5-108) could be written for this case as

\[
-0.391 = -\frac{p(1+p) (w-1)^2 w^2}{(Pw^2 + 1)^3}, \text{ where } p = 0.05.
\]

By successive approximations, one finds that a value of \( w = \frac{\mu_1}{\mu_2} = 2.621 \) satisfies this equation. The value of \( M = \frac{\mu_H}{\mu_1} \) could then be found from Equation (5-109),

\[
M = \frac{w^2 p + 1}{w(wp+1)} = 0.4532
\]

Since \( \mu_H = 1780 \text{ cm}^2/\text{volt sec} \), as shown in Table (8-1), then at room temperature this sample has

\[
\mu_1 = 3930 \text{ cm}^2/\text{volt sec}.
\]

and

\[
\mu_2 = \frac{\mu_1}{w} = 1500 \text{ cm}^2/\text{volt sec}.
\]

This shows that the mobility of the (000) conduction band is much larger than the measured \( \mu_H \).

The electron densities for this sample could now be obtained from Equations (5-112) and (5-113)

\[
n_1 = \frac{\sigma_0}{e|\mu_1| \left[ 1 + \frac{1}{Pw} \right]} = \frac{10^{19}}{3.553 (1.6) \left[ 1 + \frac{1}{Pw} \right] 3930}
\]

\[
= 5.186 \times 10^{13} \text{ cm}^{-3}
\]
and \( n_2 = \frac{n_1}{p} = n_1(20) = 1.04 \times 10^{15} \text{ cm}^{-3} \).

Most of the electrons at this temperature belong to the <100> conduction valleys. The value of \( n_2 \) obtained above compares favorably with the electron density \( n_H \) obtained from Hall coefficient in the limit of zero magnetic field. From Table (8-1), \( n_H = 8.86 \times 10^{14} \text{ cm}^{-3} \) for this sample at room temperature.

8.5 Temperature Dependence of the Resistivity, Hall Coefficient and the Mobility.

The temperature dependence of the resistivity and Hall coefficient for sample \( \text{GaAs}_{0.60} \text{P}_{0.40} \) is shown in Figure (8-13). The Hall mobility for this sample was calculated from \( \mu_H = \frac{R_H}{\rho} \) and Figure (8-14) shows its temperature dependence.

In the results shown in Figure (8-13), the effect of the <100> conduction band could be neglected at a temperature of 77°K or less for this sample. This is due to the vanishing number of electrons in this band as the temperature decreases below 77°K, as can be seen from Figure (8-1), and also due to the fact that the mobility of <100> electrons is lower than that of the (000) electrons.

In the temperature range 16°K < T < 50°K, the electrons acquire enough energy to populate the (000) conduction band. The ionization energy could be estimated from the slope of Hall coefficient variation in this range since \( n \sim e^{-\frac{E_d}{kT}} \) and hence \( R_H \sim e^{\frac{E_d}{kT}} \). \( E_d \) calculated for this sample was found to be
where $T$ is the temperature in $°K$.

Figure (8-13): Resistivity and Hall coefficient versus temperature for sample 18 GaAs.
Figure (8-14). Temperature dependence of Hall mobility for sample 18 GaAs$_{0.60}$P$_{0.40}$. The linear relationship is given by $\mu_H \propto T^{-\frac{3}{2}}$. 
\[ E_d = k \frac{\ln (6.2 \times 10^3) - \ln (1.2 \times 10^3)}{0.060 - 0.020} \]

= 0.0036 ev.

There are no published values for ionization energy of Te in GaAs \(_{1-x}P_x\) for \(x\) about 0.4. Some values\(^{24,26}\) of this energy were published for higher values of \(x\).

As the temperature increases above 50\(^\circ\)K, the electrons will be energized to the \(<100>\) valleys and the behavior of the 2-band semiconductor will appear. This is shown by the increased Hall coefficient for \(T > 140\(^\circ\)K,\)

\[-3/2\]

The mobility varies as \(T^{-3/2}\) near room temperature indicating acoustical phonon scattering. The temperature dependence of the Hall mobility of this sample is shown in Figure (8-14).
CHAPTER IX

SUMMARY

In this dissertation, the electrical properties of n-type GaAs$_{1-x}$P$_x$ are discussed. The dependence of these properties on the electron densities and mobilities in the $\Gamma$ and $X$ conduction band is investigated.

Chapter 1 discusses some of the properties of the gallium arsenide phosphide system. In Chapter 2, the energy band structure of this system is presented and the values of related effective masses and energy gaps are discussed. Chapter 3 includes the effect of impurities in GaAs$_{1-x}$P$_x$ and expressions relating the electron densities to the ionization energies, impurity atoms concentrations and temperature.

A review of the electrical transport theory for a cubic semiconductor is presented in Chapter 4. The application of this theory to the case of GaAs$_{1-x}$P$_x$ is shown in Chapter 5, where the two conduction bands are considered simultaneously and expressions for the conductivity, Hall coefficient and magnetoresistance are derived. Methods for the determination of the electron density and mobility of each band are discussed. The different scattering mechanisms which are important for this alloy are discussed in Chapter 6. In Chapter 7, the sample preparation and the experimental set up are described. Finally, the results are presented and discussed in Chapter 8.

Figure (8-1) shows the variation of the electron density ratio $\frac{n_2}{n_1}$ with $x$ at 297°K and 77°K. The magnetoresistance is found to obey the
classical analysis presented in Chapters 4 and 5, except that:

a) some samples of \( x < 0.44 \), showed a longitudinal magnetoresistance

b) the transverse magnetoresistance was found negative for small fields at 77°K for some samples.

It is suspected that the above exceptions are due to inhomogeneity in the charge carrier distribution.

Seitz magnetoresistance coefficients were evaluated for \( x \) near 0.44 and the existence of \(<100>\) spheroidal valleys in the conduction band of this alloy was proved. The effective mass ratio of these valleys is estimated to be \( K = 1.81 \). For such low value of the mass ratio, the relaxation time could be assumed isotropic. This is usually accepted for the case of III-V compounds and alloys.

From the variation of the Hall coefficient with the magnetic field, the electron densities and mobilities were determined for a sample of \( x = 0.4314 \) at room temperature.

Finally, the temperature dependence of the resistivity, Hall coefficient and mobility is presented and discussed in Section 8.5 for a sample of \( x = 0.4 \) and Te- doped. For this sample, the ionization energy is found to be 0.0036 eV.
LIST OF REFERENCES


(4) S. I. Novikova, Chapter 2, ibid.

(5) U. Piesbergen, Chapter 3, ibid.


