

MEASUREMENTS OF THE MAGNETO-SEEBECK AND
NERNST-ETTINGSHAUSEN EFFECTS IN

$\text{Ga}_{1-x}\text{In}_x\text{As}$ and GaSb

by

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Dissertation submitted to the Faculty of the Graduate School
of the University of Ottawa in partial fulfillment
of the requirements for the degree

Doctor of Philosophy

1972

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Denis J.E. Demars, Ottawa 1972.

A mes parents,

et à tous ceux dont l'affection, l'amitié ou les
conseils m'ont donné l'envie d'entreprendre cette
étude et le courage de l'achever.

S O M M A I R E

Les équations générales qui décrivent les coefficients magnéto-Seebeck et Nernst-Ettingshausen transverse, dans l'hypothèse de surfaces d'énergie sphériques et de bandes non-paraboliques, ont été adaptées dans le but de pouvoir incorporer facilement dans la théorie, le modèle de Kane et une loi générale de diffusion ou un choix de mécanismes spécifiques de diffusion. Ces équations ont été développées afin de s'appliquer à des modèles décrivant le cas d'une ou de deux bandes de conduction.

Des mesures, à température ambiante, des coefficients magnéto-Seebeck et Nernst-Ettingshausen transverse ont été effectuées en fonction d'un champ magnétique, sur le système d'alliages semi-conducteurs III-V, $\text{Ga}_{1-x}\text{In}_x\text{As}$. De plus, le coefficient de Hall a été mesuré, de même que la conductivité électrique. Les résultats ont été analysés en utilisant un modèle valable dans le cas d'une bande de conduction. Le modèle de Kane décrivant la forme de la bande, nécessite la connaissance de l'énergie de la bande interdite; choisissant des valeurs connues pour celle-ci, le niveau de Fermi a été déterminé à partir de la valeur du coefficient magnéto-Seebeck dans un champ magnétique de valeur infinie, calculé en utilisant une relation empirique. La concentration des porteurs a été obtenue à partir de la valeur du coefficient de Hall dans un champ magnétique intense. La valeur de la masse effective au bas de la bande de conduction a été déterminée, connaissant le niveau de Fermi et la

concentration des porteurs. Le paramètre de diffusion a aussi été calculé à partir de la valeur du coefficient magnéto-Seebeck dans un champ magnétique nul. Afin de confirmer cette méthode, des courbes théoriques du coefficient magnéto-Seebeck ont été calculées et comparées aux résultats expérimentaux, le niveau de Fermi et le paramètre de diffusion étant considérés comme des variables. Il a été démontré que l'utilisation de la loi empirique qui détermine le coefficient magnéto-Seebeck dans un champ magnétique de valeur infinie, est tout à fait correcte. Les courbes expérimentales du coefficient Nernst-Ettingshausen transverse ont été comparées à des courbes théoriques afin d'obtenir les valeurs du niveau de Fermi et du paramètre de diffusion; la contribution des inhomogénéités à cet effet a été considérée. Puisque le paramètre de diffusion donne une bonne indication du mécanisme de diffusion prépondérant dans le cas de matériaux ayant peu de porteurs tous dans une même bande de conduction, une brève étude des mécanismes de diffusion possibles dans ce système d'alliages a été effectuée.

Les effets magnéto-Seebeck et Nernst-Ettingshausen transverse ont été mesurés dans un échantillon de GaSb de type n, dopé au tellure. Les résultats ont été analysés à l'aide de la théorie s'appliquant au cas de deux bandes de conduction. Le modèle suivant a été considéré dans l'analyse de la diffusion: bande centrée en Γ_{1c} , phonons optiques intrabandes et interbandes, impuretés ionisées, phonons acoustiques et charge d'espace; bande centrée en L_{1c} , phonons

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A B S T R A C T

General equations for the magneto-Seebeck and transverse Nernst-Ettingshausen coefficients, valid under the assumptions of spherical energy surfaces and not necessarily parabolic bands, were developed in order to be able to easily incorporate into the theory, a Kane band model and either a general scattering law or chosen specific scattering laws. This was done for both one-conduction band and two-conduction band models.

Room temperature measurements of the magneto-Seebeck and transverse Nernst-Ettingshausen coefficients were made, as a function of magnetic field, on the III-V semiconducting alloy system of $\text{Ga}_{1-x}\text{In}_x\text{As}$. In addition, the Hall coefficient was measured together with the electrical conductivity. The results were analysed on the basis of a one-conduction band model. Using known values for the energy gap needed in the Kane model, the Fermi energy was determined from the infinite-field value of the magneto-Seebeck coefficient which had been calculated using an empirical relation; the carrier concentration was calculated from the high-field value of the Hall coefficient; using these values, the bottom of the band effective mass was determined. Knowing the Fermi energy and the zero-field value of the magneto-Seebeck coefficient, the scattering parameter was also calculated. In order to check this method of approach, the experimental curves of the magneto-Seebeck

coefficient were fitted with the Fermi energy and the scattering parameter as variables. It was shown that the empirical law used to determine the infinite-field value of the magneto-Seebeck coefficient is quite satisfactory.

The experimental curves of the transverse Nernst-Ettingshausen coefficient were fitted to yield values of the Fermi energy and of the scattering parameter, account being taken of the contribution to this effect from the inhomogeneities. The scattering index being a good indication, in the case of single band materials, of the scattering mechanism present, a brief study of the possible scattering mechanisms in this alloy system was then made.

The magneto-Seebeck and transverse Nernst-Ettingshausen effects were also measured on a sample of n-type, tellurium doped, GaSb. The results were analyzed in terms of a two-conduction band model. The analysis included the following scattering mechanisms: for the central band, Γ_{1c} , intraband and interband polar optical, ionized impurity, acoustic and space-charge; for the next higher band, L_{1c} , intraband and intervalley polar optical, acoustic and ionized impurity. With these chosen scattering laws and the band parameters determined from electrical transport work (Basinski, 72B1), good agreement was obtained between the experimental and theoretical curves without the use of any adjustable parameters.

A Monsieur J.C. Woolley,
Directeur,
Département de Physique
à l'Université d'Ottawa,
Directeur du Laboratoire
de Physique du Corps Solide.

qui m'a fait l'honneur d'assumer la
direction scientifique de cette thèse.

En témoignage de mon profond respect
et de ma gratitude.

*A Monsieur J. Basinski,
Attaché de Recherche à
l'Université d'Ottawa.*

*dont la compétence scientifique et la collaboration
amicale ont rendu possible une partie de ce travail.*

A Monsieur G. Dionne,
Chargé de Recherche à l'I.R.E.Q.

à qui j'exprime toute mon amitié.
C'est un grand plaisir pour moi de le
remercier pour de nombreuses et fructueuses
discussions.

Mes remerciements

*A tous les techniciens de l'Atelier de Mécanique,
qui ont réalisé avec habileté et compétence, les
pièces nécessaires aux différents montages utilisés.*

*A Mademoiselle D. Dubé,
qui s'est occupé avec soin, gentillesse et beaucoup
de patience, de la dactylographie de ce manuscrit.*

*Au Conseil National de Recherches et aux Gouvernements
de l'Ontario et du Québec, pour l'aide financière.*

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CHAPTER 1

INTRODUCTION

The research described in this thesis is a result of the analysis of room temperature measurements made on the semiconducting alloy system of $\text{Ga}_x\text{In}_{1-x}\text{As}$ and on the compound GaSb.

Two physical phenomena have been dealt with, the magneto-Seebeck effect and the Nernst-Ettingshausen effects. These are defined in chapter 2 together with the other thermomagnetic effects. For completeness, the thermoelectric and galvanomagnetic effects are also mentioned.

A bibliography of the literature related to those effects is not included here; rather, references to the work by other authors will be made when directly related to the present one. Extensive reviews written on the theory and the experimental results of the thermoelectric and thermomagnetic effects can be found in many text-books; for example, D.K.C. MacDonald (62M1), J. Tauc (62T1), A.C. Beer (63B1), I.M. Tsidil'kovski (62T2), O. Madelung (64M1) and Harman and Honig (67H1).

Only a few words about the usefulness of the thermoelectric and thermomagnetic effects will make it obvious why these effects have always been of interest to scientists. The sign alone, of the longitudinal and transverse N.-E. effects, gives information as to the type of scattering occurring in the material studied. The magneto-Seebeck effect in an infinite magnetic field provides with the position of the Fermi level independently of the effective mass and of the type of scattering. The

Seebeck effect is related to the type of scattering and to the Fermi level; if one is known, the other can be found. Information on the non-parabolicity of the bands can also be found by measuring the magneto-Seebeck coefficient as a function of carrier concentration. Furthermore, the thermoelectric effects form the basis for thermoelectric heat pumps and thermoelectric power generation devices. In the last few years, the phonon drag effect has aroused considerable interest in the thermoelectric effects.

Most of this will become obvious as the equations are written down, except for the phonon drag effect which is a low temperature effect.

In order to arrive at a good understanding of the phenomena studied, a derivation of the transverse N.-E. effect from first principles, using a phenomenological approach and irreversible thermodynamics, is included in chapter 3. This was felt necessary because the general equations do not make it possible to see how the different variables (e.g. relaxation time) affect or are related to the measured coefficients. Also, from that derivation, physical insight is sought by discussing the steps of that same derivation. Although it may seem a simplified description to the expert in the field, still it will be found useful and interesting.

The general theory applied in this "mémoire" is dealt with in chapter 4.

Chapter 5 describes the experimental system and all the related techniques.

The research resulting from the measurements on $\text{Ga}_{1-x}\text{In}_x\text{As}$ and on GaSb is included under chapters 6 and 7.

Chapter 6 gives an account of how one arrives at calculations of the Fermi level, the bottom of the band effective mass and the scattering parameter (section 6.3.1.). A parallel method of analysis, section 6.3.2., was necessary in order to interpret the transverse N.-E. measurements. The possible scattering mechanisms in $\text{Ga}_{1-x}\text{In}_x\text{As}$, suggested by the values of the scattering parameter were investigated in section 6.3.3., by including in the analysis, specific relaxation times.

In chapter 7, the measurements of the magneto-Seebeck and N.-E. effects on GaSb are analyzed using a two-band theory taking into account the non-parabolicity of the Γ_{1c} band. Such a theory is applied for the first time. Chosen relaxation times for both the Γ_{1c} band and the L_{1c} band are introduced and discussed.

This research project originated as one aspect of the research under way in the semiconductor group at the Physics Department of this University; this group is headed by Dr. John C. Woolley. For that reason one will find in the text, references to the work of the other scientists, either in an associated or complementary way.

CHAPTER 2

DEFINITIONS, TERMINOLOGY

AND CONVENTIONS ADOPTED

Before progressing any further, it is essential to define the effects discussed herein, so as to assign to each of them a terminology. This is needed because the same effects bear different names from one author to another.

There exists three thermoelectric phenomena in zero magnetic field and four magnetothermoelectric phenomena.

2.1. THERMOELECTRIC PHENOMENA

The Seebeck effect involves the voltage produced in a circuit consisting of two different materials when the two junctions between the materials are at different temperatures. The Seebeck coefficient α is defined as the limit of the quotient of the voltage generated in the circuit, divided by the temperature difference as the temperature difference approaches zero.

$$\alpha_{12} = \lim_{\Delta T \rightarrow 0} - \frac{\Delta V}{\Delta T} \quad 2.1$$

The Peltier effect is related to the heat which is absorbed or given off when a current passes through a junction between two different materials. The Peltier coefficient Π is defined as the quotient

of the heat absorbed by the junction, divided by the current flowing through the junction.

The third effect is the Thomson effect, a bulk effect, which is related to the absorption or evolution of heat from a material which has an electric current flowing through it and a temperature gradient along it. The Thomson coefficient τ_{Th} is the quotient of the rate of heat absorption per unit volume, divided by the product of the current density times the temperature gradient.

The Peltier and Thomson coefficients are difficult to measure; for that reason the Seebeck coefficient is usually measured and if needed, the two others are calculated from it, using the equations known in thermodynamics as the Kelvin (Thomson) relations.

In this thesis, only the Seebeck coefficient will be dealt with, the others having been defined to exclude any misinterpretation of the terminology.

There are two methods of defining the Seebeck coefficient (thermoelectric power) of a single material: either one uses the Kelvin relations in an integrated form and measures the Thomson coefficient, or the relative coefficients are defined as the coefficients of a couple composed of the material and a standard reference material such as platinum or lead. The standard reference material is sometimes called the "passive element"; it could also consist of a material with a negligible thermoelectric power as compared to that of the other material. The latter convention is used here and discussed in chapter 5.

The magneto-Seebeck coefficient $\alpha(B)$ is accordingly the value of the Seebeck coefficient in a magnetic field of induction B .

2.2. THERMOMAGNETIC PHENOMENA

These will be defined with the aid of figure 2.1. A right-handed system of coordinates x , y and z is used as shown.

The thermomagnetic effects will appear in semiconductors subjected to a longitudinal temperature gradient $\partial T/\partial x$ and a transverse magnetic field of induction B_z . These effects, also known as magneto-thermal effects, are analogues of magnetoelectric phenomena and in both cases one distinguishes transverse (odd) and longitudinal (even) effects. The transverse effects are those which appear in the direction normal to the primary heat flow. The longitudinal effects are those which appear parallel to the primary heat flow.

In a longitudinal magnetic field, that is, in a field parallel to the heat flow, no thermomagnetic effects appear in isotropic semiconductors. The longitudinal effects mentioned above, which appear in a transverse magnetic field, have to be discerned from those which appear in a longitudinal magnetic field only in semiconductors in which the effective mass and the relaxation time of carriers are not independent of the direction and are given by tensors instead of by scalars.

Of the four thermomagnetic effects, two of them are transverse and two are longitudinal. The transverse N.-E. effect is the

appearance of a transverse potential difference. The Righi-Leduc effect is observed as a transverse temperature difference. In the longitudinal N.-E. effect, a resultant longitudinal potential difference is observed as a change in the thermoelectric power. In the Magghi-Righi-Leduc effect, a resultant longitudinal temperature difference is observed as a change of the thermal conductivity in a magnetic field.

These effects can be described in an analytical form in the following way:

2.2.1. Longitudinal N.-E. effect

Referring to figure 2.1.a:

$$E_x(B) - E_x(o) = - \frac{\partial V}{\partial x} = [\alpha(B) - \alpha(o)] \frac{\partial T}{\partial x} \quad 2.2$$

The sign of this effect is chosen in this thesis on the basis of the following:

$$\Delta \alpha(B) = | \alpha(B) | - | \alpha(o) | \equiv Q_{//}(B) \quad 2.3$$

where $Q_{//}$ is the longitudinal N.-E. coefficient and $\alpha(B)$, $\alpha(o)$ are the thermoelectric powers with and without a magnetic field. $Q_{//}$ is therefore positive if the absolute value of the thermoelectric power increases in a magnetic field. This definition using absolute values is quite useful because it makes $Q_{//}$ independent of the sign of the carrier. That is the case for the transverse N.-E. effect as will be seen later on.

Note the terminology up to now:

Seebeck effect: thermoelectric power, α .

Magneto-Seebeck effect: value of α in a magnetic field of induction B , $\alpha(B)$.

Longitudinal N.-E. effect: the variation of the absolute value of the thermoelectric power in a magnetic field.

2.2.2. Transverse N.-E. effect

If a temperature gradient and a magnetic field, mutually perpendicular, are applied to a sample, figure 2.1.b, an electric field E_y will result with the value:

$$E_y = - \frac{V_y}{a} = Q_L B_z \frac{\partial T}{\partial x} \quad 2.4$$

The transverse N.-E. coefficient is therefore:

$$Q_L = \frac{- V_y}{a \cdot B_z \cdot \partial T / \partial x} \quad 2.5$$

where a is the width of the sample. We then have:

$$Q_L = \frac{- V_y \cdot \text{Length}}{\text{width} \cdot B_z \cdot (T_2 - T_1)} \quad 2.6$$

where T_1 and T_2 are the temperatures at the cool end and at the warm end of the sample respectively.

The effect will be said to be positive if a positive temperature gradient along the x -axis and the positive magnetic field

along the z-axis produce a positive electric field E_y along the y-axis.

It turns out that the utilisation of the conventions described for these two effects is very convenient in the analysis of data. Both $Q_{\perp}$ and $Q_{//}$ are independent of the sign of the carriers; they will therefore have the same sign, indicating the possible nature of the scattering mechanism present in the material investigated.

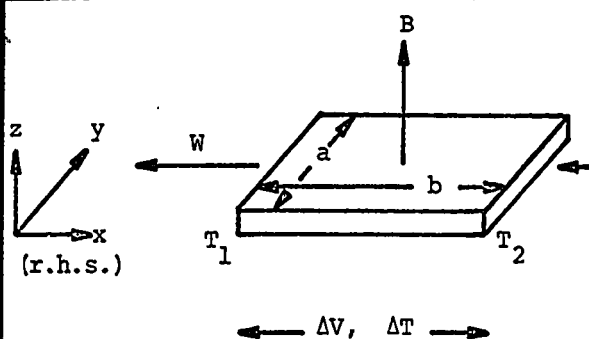
2.2.3. Others

As for the other effects described in figure 2.1, drawings c and d, S is the Righi-Leduc coefficient; λ_0 and λ_B are the thermal conductivities in the absence and in the presence of a magnetic field; A is the Magghi-Righi Leduc coefficient.

Three of these thermomagnetic effects can be either isothermal with $\partial T/\partial y = \partial T/\partial z = 0$, or adiabatic with no transverse heat flows W_y and W_z . Obviously, the Righi-Leduc effect cannot be isothermal.

2.3. GALVANOMAGNETIC EFFECTS

These effects are now very well known. A brief description is given in figure 2.2. If a current I_x is flowing in a sample and the magnetic field is applied, a transverse voltage, the Hall voltage will appear. At the same moment, a transverse temperature gradient will also

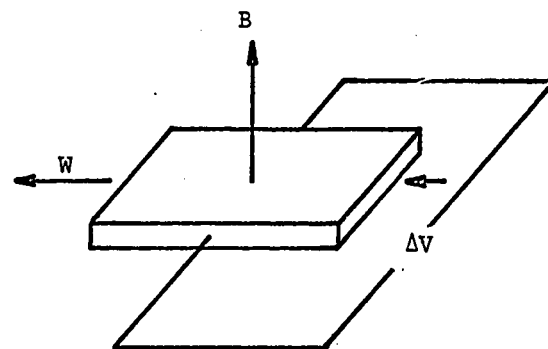


$$\alpha(o) = -[\Delta V(o)/\Delta T] = (E_x(o) \cdot b/\Delta T)$$

$$\alpha(B) = -[\Delta V(B)/\Delta T] = (E_x(B) \cdot b/\Delta T)$$

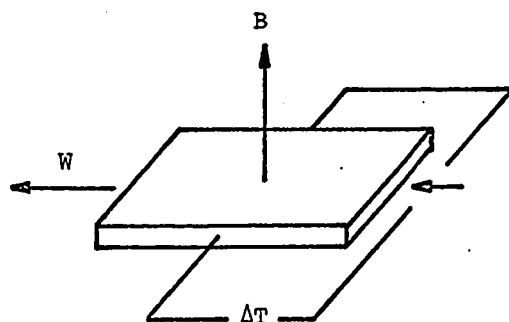
$$|\alpha(B)| - |\alpha(o)| = \Delta\alpha(B) \equiv Q_{//}$$

a. Longitudinal Nernst-Ettingshausen Effect



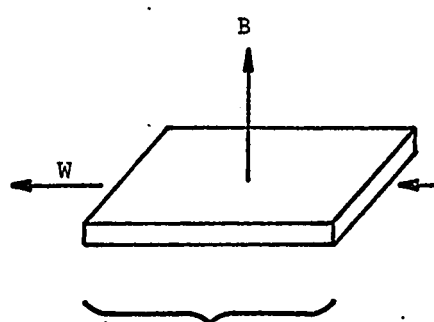
$$E_y = -\Delta V/a = Q_{\perp} B_z (\partial T/\partial x)$$

b. Transverse N.-E. Effect (Nernst Effect)



$$\partial T/\partial y = \Delta T/a = S B_z (\partial T/\partial x)$$

c. Righi-Leduc Effect



$$\Lambda = (\lambda_o - \lambda_B)/\lambda_o$$

d. Magghi-Righi-Leduc effect (Change of thermal conductivity)

Note. 1) The effect is ISOTHERMAL if there are no transverse temperature gradients along the y- and z-axes: $\partial T/\partial y = \partial T/\partial z = 0$.

2) The effect is ADIABATIC if there are no transverse heat flows:

$$W_y = W_z = 0.$$

Figure 2.1 Thermomagnetic phenomena

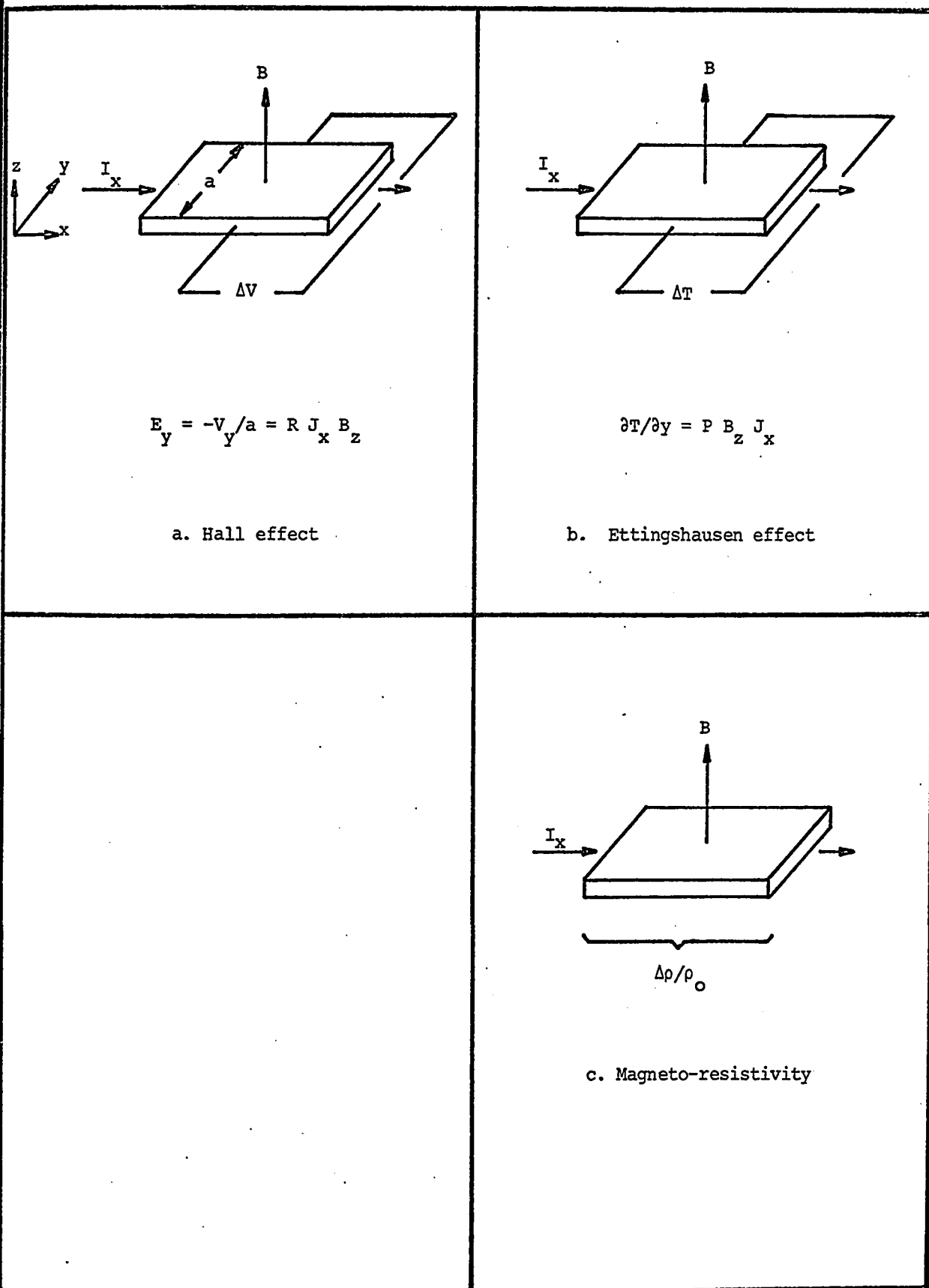


Figure 2.2 Galvanomagnetic effects

arise; this is the Ettingshausen effect. Because the current carriers are now deflected with respect to the x-axis, the resistance in the x-direction will change giving rise to what is termed the magnetoresistance.

Now that all the analytical definitions are given, chapter 3 will present, mainly, a derivation of the transverse N.-E. effect. This effect is chosen because, as the equations are laid out, one can see what is happening in the material microscopically. The other effects can easily be understood by extrapolation.

CHAPTER 3

GENERAL NOTIONS ON THE THERMOMAGNETIC

EFFECTS AND POINTS OF INTEREST

The aim of this chapter is to arrive at a basic physical understanding of the phenomena studied; it does not contain a derivation of the formulae used in this thesis but rather, a special case of those to which they reduce if the band structure is of a parabolic type. Both are for spherical energy surfaces.

Thermodynamics is used in order to arrive at the equations describing the current densities due to the potential and thermal gradients. This is parallel to the use of a kinetic theory. Scalars are used instead of tensors as a simplification. Furthermore this chapter limits itself to specific cases: intrinsic and extrinsic with one type of charge carriers.

Most of the equations used here can be found in the book by Tauc (62T1); they have been arranged in a logical manner to serve the purpose of this chapter and comments are added.

Simple physical models describing microscopically the effects are included.

3.1. CURRENT DENSITIES ARISING IN THE PRESENCE OF AN ELECTRIC POTENTIAL GRADIENT AND A THERMAL GRADIENT

Let it be assumed that the system can be analyzed into macroscopically small regions where the thermodynamic variables can be defined and considered as constants; e.g. temperature, chemical potential etc.

It is also supposed that an electric potential gradient, $\text{grad } \phi$, and a thermal gradient, $\text{grad } T$, exist in the material.

It is well known in thermodynamics that if a phenomenon is irreversible, there is a creation of entropy; this will be used as a starting point. One cannot write any longer that :

$$dS = dQ/T \quad 3.1$$

where dS is the entropy increment, dQ the quantity of heat input.

The entropy is expressed in such a case as:

$$dS > dQ/T \quad 3.2$$

After having calculated the quantity of created entropy, with the aid of a system of currents and conjugated forces to those currents, following a method by Onsager, the electric and thermal current densities will be expressed in terms of linear relations of $\text{grad } \phi$ and $\text{grad } T$.

Introducing entropy into the problem by using Gibbs' relation, one is able to show that the entropy created per second per cm^3 is:

$$\frac{1}{T} \left[J_n \text{ grad } \phi - J_N T \text{ grad } \frac{\zeta'_n}{T} - \frac{Q}{T} \text{ grad } T \right] \quad 3.3$$

where J_n : electric current density
 Q : thermal current density
 J_N : $J_n / -e$ is a particle current density
 ζ'_n : chemical potential relative to some arbitrary reference.

Onsager suggests that this created entropy should be expressed in the form:

$$\sum_i I_i X_i \quad 3.4$$

I_i : currents
 X_i : conjugated forces to each current.

and

$$I_i = \sum_{j=1}^n a_{ij} X_j \quad (\text{Onsager relations}) \quad 3.5$$

with $a_{ij} = a_{ji} \quad (\text{Onsager theorem}) \quad 3.6$

The current densities are therefore expressed as follows:

$$J_N = \frac{J_n}{-e} = a_{11} (-e \text{ grad } \phi + T \text{ grad } \frac{\zeta'_n}{T}) + a_{12} \frac{1}{T} \text{ grad } T \quad 3.7$$

and

$$Q = a_{21} (-e \text{ grad } \phi + T \text{ grad } \frac{\zeta'_n}{T}) + a_{22} \frac{1}{T} \text{ grad } T \quad 3.8$$

It is easy to deduce that $a_{11} = \frac{\sigma_n}{e}$ where σ_n is the electrical conductivity due to the electrons. Also, $a_{22} = K_n T$, K_n being the thermal conductivity. Dividing equation 3.8 by equation 3.7 and setting $\text{grad } T = 0$:

$$\frac{a_{21}}{a_{11}} = \frac{a_{12}}{a_{11}} = \frac{Q}{J_N} = Q_n^* \quad 3.9$$

Where Q_n^* is the average quantity of heat carried by each particle.

Replacing a_{11} and a_{12} in equation 3.7, the electric current density is:

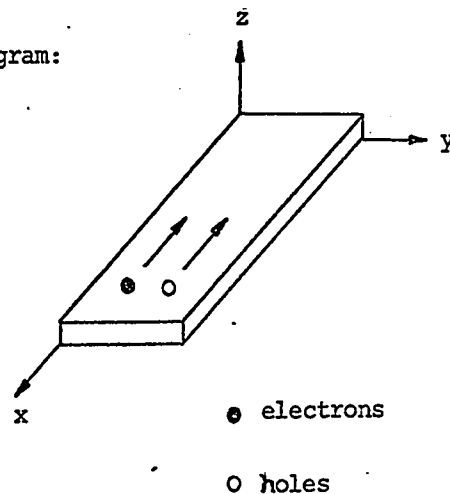
$$J_n = \frac{\sigma_n}{e} \left[-e \text{ grad } \phi + T \text{ grad } \frac{\zeta'_n}{T} + Q_n^* \frac{1}{T} \text{ grad } T \right] \quad 3.10$$

The same equations apply to J_p , subscript n being replaced by p .

3.2. THERMOELECTRIC POWER AND INTRINSIC TRANSVERSE N.-E. EFFECT

Consider the following diagram:

The heat applied at the high x end of the sample creates pairs of electrons and holes. This gives rise to the current densities J_{nx} and J_{px} .



These current densities compensate each other mutually so that:

$$J_{nx} + J_{px} = 0 \quad 3.11$$

Using equation 3.10 and the similar one for J_{px} , one solves for $\text{grad } \phi$.

$$E_x = -\text{grad } \phi = -\frac{1}{e} t_n \frac{d\zeta'_n}{dx} - \frac{1}{e} t_p \frac{d\zeta'_p}{dx} - \frac{1}{e} (t_n S_n^{*'} - t_p S_p^{*'}) \frac{dT}{dx} \quad 3.12$$

where

$$t_n = \frac{\sigma_n}{\sigma}, \quad t_p = \frac{\sigma_p}{\sigma} \quad \text{with } \sigma = \sigma_n + \sigma_p,$$

and

$$S_n^{*'} = \frac{1}{T} (Q_n^{*'} - \zeta'_n) \quad 3.13$$

$$S_p^{*'} = \frac{1}{T} (Q_p^{*'} - \zeta'_p) \quad 3.14$$

$S_n^{*'}$ stands for the entropy transferred by one electron per cm^2 . per sec.

It is independent of the zero energy level selected.

The thermoelectric power α has been defined as:

$$\alpha = \lim_{\Delta T \rightarrow 0} - \frac{\Delta V}{\Delta T}$$

where

$$\Delta V = \int_0^L -E_x dx$$

If ΔT is small compared with the temperature at which the measurements are made, then:

$$\frac{d\zeta'_n}{dx} = \frac{d\zeta'_p}{dx} = 0$$

One obtains for α :

$$\alpha = -\frac{1}{e} (t_n S_n^* - t_p S_p^*) \quad 3.15$$

For an n-type semiconductor, when $\sigma_p = 0$:

$$\alpha_n = -\frac{1}{e} t_n S_n^* = -\frac{S_n^*}{e} \quad 3.16.a$$

$$= \frac{k}{e} \frac{(\zeta_n - Q_n^*)}{kT} \quad 3.16.b$$

where ζ_n is the chemical potential w.r.t. the bottom of the conduction band ($\zeta_n' = \zeta_n + E_c$). Considering only equation 3.16.b, the thermoelectric power clearly depends on the sum of the potential energy ζ_n and the kinetic transport energy Q_n^* provided by the heat source.

In semiconductors where the position of the Fermi level is inside the band gap, the absolute values of both these energies are additive; the thermoelectric power is therefore large. When the Fermi level is in the conduction band the difference between ζ_n and Q_n^* is smaller and the thermoelectric power decreases; this is why the thermoelectric power decreases as the carrier concentration increases. This also explains why metals have a low thermoelectric power by comparison to that of semiconductors.

The thermoelectric power could also be qualified by saying that it is a current of entropy, carried from the warm end to the cool end of the sample; see equation 3.16.a.

The intrinsic transverse N.-E. effect is easy to understand; replacing $\text{grad } \phi$, equation 3.12, in equation 3.10 for J_{nx} and in a similar equation for J_{px} one obtains:

$$J_{nx} = -J_{px} = \sigma \frac{k}{e} t_n t_p [(Q_n^* + Q_p^* + E_G)/kT] \text{ grad } T \quad 3.17$$

If a weak magnetic field of induction B_z is applied, it will deflect J_{nx} by an angle θ_n and J_{px} by an angle θ_p . Assuming that θ_n and θ_p are small:

$$J_y = -\theta_n J_{nx} - \theta_p J_{px} \quad 3.18$$

$$J_y = (\theta_p - \theta_n) J_{nx} \quad 3.19$$

$$= (\mu_{nH} + \mu_{pH}) B_z J_{nx} \quad 3.20$$

To balance out this current, the field E_y is required:

$$J_y = -\sigma E_y \quad 3.21$$

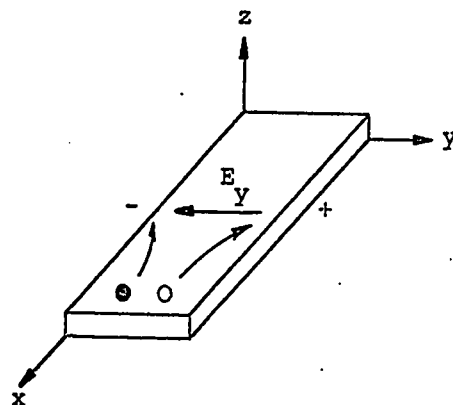
One obtains for the transverse N.-E. coefficient:

$$Q_{\perp} = \frac{E_y}{B_z \cdot \partial T / \partial x} = \frac{k}{e} t_n t_p \left[\frac{E_G + Q_n^* + Q_p^*}{kT} \right] (\mu_{nH} + \mu_{pH}) \quad 3.22$$

From this last equation, $Q_{\perp}$ is seen to be independent of the magnetic field induction in the weak field region.

From the following diagram:

the coefficient Q_1 is obviously
always negative for intrinsic
material.



Note that if in equation 3.22, $t_p = 0$, the coefficient Q_1 becomes equal to zero. This is not true; therefore, for the extrinsic case of the transverse N.-E. effect, a different approach has to be used.

3.3. EXTRINSIC TRANSVERSE N.-E. EFFECT (n-type)

This is by far the most interesting of the thermomagnetic effects.

So that this effect is not predicted, by the theory, to be equal to zero, the action of the magnetic field has to be considered on dJ_{nx} and not on J_{nx} .

If one applies heat to one end of a sample and a weak magnetic field of induction B_z , fast electrons will go down the temperature gradient, hence building up an electric field $-E_x$ along the x-axis; then, slow electrons will come back due to this electric field $-E_x$. Both, fast and slow electrons will be deviated by the magnetic field. If they possess the same relaxation time, no transverse voltage will develop; on the other hand if the relaxation time depends on energy, a transverse potential difference will build up.

The current density J_{nx} needs to be expressed in terms of

τ . One has to substitute Q_n^{*1} and σ_n in equation 3.10.

$$Q_n^{*1} = \frac{\langle \tau \epsilon_n^2 \rangle}{\langle \tau \epsilon_n \rangle} + E_c \quad 3.23$$

(See Appendix 3.1)

$$\sigma = ne\mu = \frac{ne^2}{m_n} \frac{\langle \tau \epsilon_n \rangle}{\langle \epsilon_n \rangle} \quad 3.24$$

where ϵ_n is the energy and m_n is the effective mass.

At thermal equilibrium $J_{nx} = 0$. Equation 3.10 becomes:

$$J_{nx} = \frac{en}{m_n} \frac{\langle \tau \epsilon_n \rangle}{\langle \epsilon_n \rangle} \left[eE_x + T \frac{d}{dx} \left(\frac{\zeta_n}{T} \right) \right] + \frac{en}{m_n} \frac{\langle \tau \epsilon_n^2 \rangle}{\langle \epsilon_n \rangle} \frac{1}{T} \frac{dT}{dx} = 0 \quad 3.25$$

If one solves for the term in brackets,

$$eE_x + T \frac{d}{dx} \left(\frac{\zeta_n}{T} \right) = - \frac{\langle \tau \epsilon_n^2 \rangle}{\langle \tau \epsilon_n \rangle} \frac{1}{T} \frac{dT}{dx} \quad 3.26$$

The current density with electrons having an energy

between ϵ_n and $\epsilon_n + d\epsilon_n$ is:

$$dJ_{nx} = \frac{edn}{m_n} \frac{\tau \epsilon_n}{\langle \epsilon_n \rangle} \left[- \frac{\langle \tau \epsilon_n^2 \rangle}{\langle \tau \epsilon_n \rangle} \frac{1}{T} \frac{dT}{dx} \right] + \frac{edn}{m_n} \frac{\tau \epsilon_n^2}{\langle \epsilon_n \rangle} \frac{1}{T} \frac{dT}{dx} \quad 3.27$$

In equation 3.27, $\langle \epsilon_n \rangle$ is only a normalizing factor.

The term inside the parentheses represents the force acting on the

electrons and therefore retains its brackets.

Finally:

$$dJ_{nx} = \frac{edn}{m_n} \left[\frac{\tau_n \epsilon_n^2}{\langle \epsilon_n \rangle} - \frac{\tau_n \epsilon_n}{\langle \epsilon_n \rangle} \frac{\langle \tau_n \epsilon_n^2 \rangle}{\tau_n \epsilon_n} \right] \frac{1}{T} \frac{dT}{dx} \quad 3.28$$

The electrons represented by equation 3.28 will undergo a rotation through an angle θ such that:

$$dJ_{ny} = \omega_B \tau_n dJ_{nx} \quad (\text{for small } B \text{ only}) \quad 3.29$$

The total current density, hence, is:

$$J_{ny} = \frac{eB_z}{m_n} \int_0^{J_{nx}} \tau_n dJ_{nx} \quad 3.30$$

$$J_{ny} = \left(\frac{e}{m_n}\right)^2 B_z \frac{n}{T} \frac{dT}{dx} \left[\frac{\langle \tau_n^2 \epsilon_n^2 \rangle}{\langle \epsilon_n \rangle} - \frac{\langle \tau_n^2 \epsilon_n \rangle}{\langle \epsilon_n \rangle} \frac{\langle \tau_n \epsilon_n^2 \rangle}{\tau_n \epsilon_n} \right] \quad 3.31$$

$$= -\sigma E_y \quad 3.32$$

The coefficient Q_1 is:

$$Q_1 = \frac{1}{m_n T} \left[\langle \tau_n^2 \epsilon_n \rangle \frac{\langle \tau_n \epsilon_n^2 \rangle}{\langle \tau_n \epsilon_n \rangle^2} - \frac{\langle \tau_n^2 \epsilon_n^2 \rangle}{\langle \tau_n \epsilon_n \rangle} \right] \quad 3.33$$

The sign of Q_1 extrinsic is therefore completely determined by the relation of τ with the energy. This is a most important result.

When the relation $\tau = \tau_0 \epsilon_n^s$ can be used, equation 3.33 reduces to:

$$Q_1 = - \frac{k}{e} \mu_{nH} s \quad 3.34$$

For acoustic scattering, $s = -1/2$, Q_1 is positive

For ionized impurity scattering, $s = +3/2$, Q_1 is negative

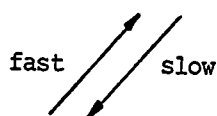
If τ is independent of ϵ , $Q_1 = 0$.

Since the sign of Q_1 (extrinsic) is positive in the case of scattering on the thermal vibrations of the lattice, in this case, the effect can be used to find out when the material will become intrinsic. The sign is negative for intrinsic material.

3.4. PHYSICAL INTERPRETATION

3.4.1. Transverse N.-E. Effect (Extrinsic)

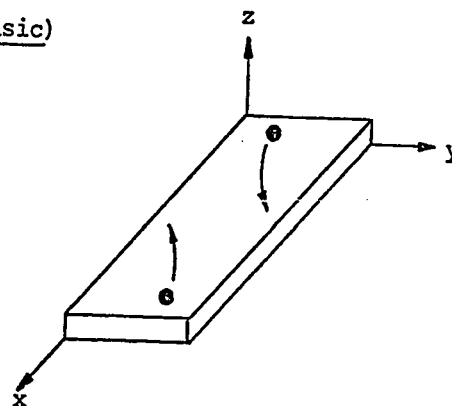
There are two typical currents of electrons:



under the condition $J_{nx} = 0$.

The angle θ_i through which each of those currents will be deflected is

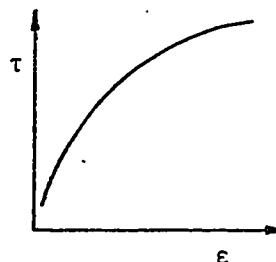
$$\theta_i = \omega \tau_i = \frac{eB_z}{m_n} \tau_i \quad 3.35$$



It is seen to be independent of the velocity of the electrons.

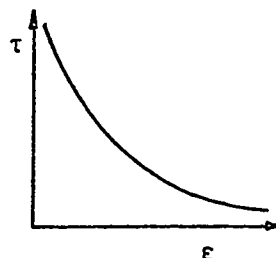
Therefore for a constant relaxation time, no transverse voltage will develop in weak fields. However, if ionized impurity scattering dominates:

The fast electrons will be more deviated so that the resultant electric field along the y-axis will be negative ($- \leftarrow +$)
 E_y



If the scattering is of the thermal vibration type:

The fast electrons will be less deviated and the resultant electric field E_y will change sign so that the coefficient Q_1 is positive.



3.4.2. Other thermomagnetic effects

If the fast electrons are those that are more deflected, they will lose entropy to the left side (negative y-direction) of the sample, producing a transverse thermal gradient (Righi-Leduc effect) and a decrease in the thermoelectric power (longitudinal N.-E. effect).

As in the case of magnetoresistance, the electrons then have a shorter mean-free path component along the x-axis; this leads to a change in the thermal conductivity (Magghi-Righi-Leduc effect).

CHAPTER 4

THEORY

The general equations to be given in sections 4.1 and 4.2 can be found in Harman and Honig (67H1) chapter 5, p. 205. In section 5.13 of their volume, Harman and Honig mention a method pioneered by the Polish school of scientists, members of which are J. Kolodziejczak, L. Sosnowski, W. Zawadzki and S. Zukotynski*.

In this work, references will be made mainly to the publications published by those authors.

The reader will find in the above reference, (67H1), an outline of the kinetic theory of transport, based on the solution of the Boltzmann's equation, leading to the formulation of the equations for the magneto-Seebeck and transverse N.-E. effect to be described in the next sections.

4.1. MAGNETO-SEEBECK EFFECT

On the assumption of spherical, though not necessarily parabolic structure of the bands, Kolodziejczak (61K1) has developed the theory of some of the thermo- and galvanomagnetic effects for the general case of transport by many kinds of carriers.

* Now at the University of Toronto.

The following expression is obtained for the isothermal magneto-Seebeck effect:

$$\alpha(B) = \frac{\sum_i \sigma_{11}^i \left[\theta_{11}^i - \frac{(E_F)_i}{e_i T} \sigma_{11}^i \right] + \sum_i \sigma_{12}^i \left[\theta_{12}^i - \frac{(E_F)_i}{e_i T} \sigma_{12}^i \right]}{\left[\sum_i \sigma_{11}^i \right]^2 + \left[\sum_i \sigma_{12}^i \right]^2} \quad 4.1$$

The index "i" denotes a given energy band, e_i is the carrier charge $\pm e$ and $(E_F)_i$ the respective Fermi energies measured from the bottom of each band.

The conductivity tensors are:

$$\sigma_{11}^i = \frac{e_i^2}{3\pi^2} \left\langle \frac{\mu_i}{1 + B^2 \mu_i^2} \right\rangle$$

$$\sigma_{12}^i = \frac{e_i B}{3\pi^2} \left\langle \frac{\mu_i^2}{1 + B^2 \mu_i^2} \right\rangle$$

$\theta_{\mu\nu}^i$ is one component of the thermoelectric tensor;

$$\theta_{11}^i = \frac{k}{3\pi^2} \left\langle \frac{\xi_i \mu_i}{1 + B^2 \mu_i^2} \right\rangle$$

$$\theta_{12}^i = \frac{k_B}{3\pi^2} \left\langle \frac{\xi_i \mu_i^2}{1 + B^2 \mu_i^2} \right\rangle \quad 4.2$$

with μ_i , ξ_i and k being respectively the mobility, the reduced energy E_i/kT and Boltzmann's constant.

The bracket symbol is defined as:

$$\langle A_i \rangle \equiv \int_0^\infty \left(\frac{\partial f_0}{\partial \xi} \right)_i A_i k^3(\xi_i) d\xi_i \quad 4.3$$

where f_0 is the Fermi-Dirac distribution function and k is the wave vector depending on the assumed band structure.

In the above expressions, the mobility is

$$\mu_i = \frac{e_i \tau_i}{m_i^*} \quad 4.4$$

where τ_i is the relaxation time and m_i^* is the effective mass which enters into the transport properties of carriers in a spherical band of arbitrary shape i.e.

$$\frac{1}{m_i^*} = \frac{kT}{\hbar^2 k_i} \left(\frac{d\xi}{dk} \right)_i \quad 4.5$$

If equation 4.1 is solved for $B = 0$ and for $B = \infty$, one obtains:

$$\alpha(0) = \frac{1}{\sigma} \sum_i \frac{k}{e_i} \sigma_i \left[\frac{\langle \xi_i \mu_i \rangle}{\langle \mu_i \rangle} - \frac{(E_F)_i}{kT} \right] \quad 4.6$$

and

$$\alpha(\infty) = \frac{\sum_i k n_i \left[\frac{\langle \xi_i \rangle}{\langle 1_i \rangle} - \frac{(E_F)_i}{kT} \right]}{\sum_i e_i n_i} \quad 4.7$$

with the carrier concentration n_i being:

$$n_i = \frac{1}{3\pi^2} \int_0^\infty \left(-\frac{\partial f_0}{\partial \xi} \right)_i k^3(\xi_i) d\xi_i \equiv \frac{1}{3\pi^2} \langle 1_i \rangle \quad 4.8$$

4.2. TRANSVERSE N.-E. EFFECT

Under the same conditions as for $\alpha(B)$, the coefficient Q_1 is given by:

$$Q_1 = \frac{1}{B} \frac{\sum_{i12}^i \sigma_{i12}^i - \sum_{i11}^i \sigma_{i11}^i + \sum_{i11}^i \frac{\sum_{i12}^i \sigma_{i12}^i}{e_i T} - \sum_{i12}^i \frac{\sum_{i11}^i \sigma_{i11}^i}{e_i T}}{(\sum_{i11}^i \sigma_{i11}^i)^2 + (\sum_{i12}^i \sigma_{i12}^i)^2} \quad 4.9$$

where "i" denotes a given energy band and the tensors are identical to those defined previously.

The equations described in both sections 4.1. and 4.2. will be applied to the alloy system of $\text{Ga In}_{1-x}\text{As}$ where they are reduced to a one-band conduction case and to GaSb for the case of a two-band conduction, n-type in both instances.

4.3. BAND STRUCTURE

4.3.1. Kane Model

In the present work, a simplified version of Kane's model will be used.

A frequently used approximate solution of the Kane's equation for the conduction band is (68A1):

$$E = ak^2 + \frac{E_o^*}{2} \left[\left(1 + \frac{a\beta k^2 P^2}{E_o^*} \right)^{1/2} - 1 \right] \quad 4.10$$

where

$$a = \hbar^2/2m$$

m : electron rest mass

$P^2 \equiv$ square of a matrix element

$E_o^* \equiv$ effective mass band gap

$\beta \equiv$ parameter depending on E_o^* and Δ_o ; it is equal to 8/3 if $E_o^* \ll \Delta_o$ and to 4 if $E_o^* \gg \Delta_o$.

Δ_o is the spin-orbit splitting of the valence bands at (ooo).

It can be shown, (69A1), that equation 4.10 can be reduced to:

$$E = ak^2 + \frac{E_o^*}{2} \left\{ \left[1 + \frac{4ak^2}{E_o^*} \left(\frac{m}{m_o^*} - 1 \right) \right]^{1/2} - 1 \right\} \quad 4.11$$

where E is measured from the conduction band minimum and m_o^* is the bottom of the band effective mass.

The same relation was obtained by Cardona (61C1). If one inverts equation 4.11, $k(E)$ is obtained as:

$$k = \left(\frac{m E_o^*}{2a m_o^*} \right)^{1/2} \left[1 + \frac{2E m_o^*}{E_o^* m} - \left\{ 1 + \frac{4E m_o^*}{E_o^* m} \left(1 - \frac{m_o^*}{m} \right) \right\}^{1/2} \right]^{1/2} \quad 4.12$$

It should be noted that if $m_o^*/m \ll 1$, equation 4.11 reduces to:

$$k = \left(\frac{E m_o^*}{am} \right)^{1/2} \left(1 + \frac{E}{E_o^*} \right)^{1/2} \quad 4.13$$

and for large energy gap E_o^* and small effective mass m_o^* , equation 4.11 reduces to the standard parabolic band equation, $E = \hbar^2 k^2 / 2m^*$. In this case, the effective mass is independent of the energy.

Using equation 4.5 and 4.12, the effective mass for the case of a non-parabolic band is given by:

$$\frac{m}{m^*(k)} = 1 + \left(\frac{m}{m_o^*} - 1 \right) / \left\{ 1 + \frac{4a}{E_o^*} \left(\frac{m}{m_o^*} - 1 \right) k^2 \right\}^{1/2} \quad 4.14$$

It has been shown by Aubin (69A2), that for InSb, relation 4.11 is a good approximation to the Kane model. In the case of the compounds considered in this work, where the interaction between the valence and conduction bands is weaker, equation 4.11 is therefore expected to be an even better approximation to the Kane model.

4.3.2. Effective mass band gap

The effective mass band gap E_o^* is the value of the band gap if only lattice dilation effects are considered, after Ehrenreich (57E1). Its value lies between E_o and E_{oo} , the intrinsic band gap values at the temperature of observation and at absolute zero respectively.

It may be expressed in the form (68V1):

$$E_o^* = E_{oo} - \left(\frac{E_{oo} - E_o}{a} \right) \quad 4.15$$

where a is the parameter which determines the relative effect of lattice dilation and interaction of the phonon field on the gap.

For InSb, it was shown (62S1) that $E_o^* = 0.21$ eV, i.e. it is approximately halfway between the values of E_o and E_{oo} ; hence, in the present work, a value of $a = 2$ was chosen.

The effective mass band gap will therefore be expressed as:

$$E_o^* = (E_o + E_{oo})/2 \quad 4.16$$

4.3.3. Effective masses

The effective mass which enters into the transport properties of carriers in a spherical band of arbitrary shape is given by equation 4.5. It is seen that in general this mass depends on energy and describes the non-parabolicity of the band. This effective mass applies to InAs and GaAs both having spherical energy surfaces; only the central band in GaAs being effective at the electron concentrations dealt with, the next higher band being at 0.38 eV along the $\langle 100 \rangle$ directions (72B3).

For the case of GaSb, the central band at (000) is spherical but non-parabolic. The Kane model described above was used. The $\langle 111 \rangle$ band has a non-spherical symmetry and is parabolic. Although equations for the thermomagnetic effects have been derived for such cases, by Zukotynski and Kolodziejczak, (63Z1) and (64K1), the non-sphericity will be taken into account in the effective mass.

The conductivity effective mass,

$$\frac{1}{m_c} = \frac{1}{3} \left(\frac{1}{m_L} + \frac{2}{m_T} \right) \quad 4.17$$

is used in the mobility calculations whereas a "density of states" effective mass:

$$m_d = (m_L m_T^2)^{1/3} \quad 4.18$$

is introduced in the scattering laws describing the relaxation times.

In the above equations, m_L and m_T are respectively the longitudinal and transverse effective masses.

4.4. SCATTERING IN III-V COMPOUNDS

One has noticed in sections 4.1. and 4.2. that $\alpha(B)$ and $Q_L(B)$ are written in terms of tensors, equations 4.2. Those tensors are in turn dependent on the mobility μ defined by equation 4.4 as proportional to the relaxation time τ . It therefore, becomes obvious that in order to analyze the thermomagnetic effects, assumptions have to be made as to the scattering mechanisms occurring in the material studied.

The usual scattering mechanisms in semiconductors can be represented by expressions known as scattering laws. These give a reasonable indication of the energy and temperature dependence of the relaxation time. A derivation of those scattering laws necessitates an analysis of the scattering process itself; it will not be presented here. The scattering laws will be described for the mechanisms that are dealt with in this thesis in relation to chapters 6 or 7.

A discussion of scattering can be found in Beer (63B1) where he refers to review articles written by Brooks (p. 144, 55B1), Blatt (p. 287, 57B1) and also by Wilson (p. 251, 53W1) for information on the analysis itself.

The reader should keep in mind that the equations to be cited are derived under the assumption that the collision term in

Boltzmann's equation can be written in the form:

$$\left(\frac{\partial f}{\partial t} \right)_{\text{collision}} = - \frac{f - f_0}{\tau} \quad 4.19$$

where f_0 is the equilibrium distribution function and f is that under the applied field. This is commonly known as the relaxation time approximation as opposed to the use of a variational method to solve the Boltzmann transport equation. The validity of this assumption will be discussed later; let us say for now that if the energy absorbed or emitted by an electron is small compared with its initial energy, equation 4.19 is quite valid.

The scattering mechanisms to be discussed may be divided into two groups: lattice phonon scattering and lattice defect scattering. The first group includes acoustic and optical phonon scattering. Ionized impurity, space-charge and alloy scattering form the second group. For simplification in the indexing of the sections, they will be described in sequence.

4.4.1. Acoustic phonon scattering, "deformation potential"

Bardeen and Shockley (50B1, 50S1) derived an expression for this relaxation time describing the interaction potential involved in the scattering of a charge carrier by a lattice wave of the acoustic type in terms of the shift in energy band resulting from dilation due to the longitudinal waves.

Equation A.37 of (p. 80, 50S1) is:

$$\frac{1}{\tau_{al}} = \frac{m_e P E_1^2 k T}{\pi \hbar^4 \rho U_l^2} \quad (\text{MKS}) \quad 4.20$$

where ρ is the density, U_l is the velocity of the longitudinal waves in the crystal, P is the momentum of the charge carrier and E_1 is the deformation potential defined by

$$\Delta E_c = E_1 \frac{\Delta V}{V_0} \quad 4.21$$

Here ΔE_c is the change in energy corresponding to the bottom of the conduction band due to a small change ΔV of the original volume V_0 .

If the momentum P is replaced in equation 4.20 by $\hbar k$ and m_e taken as the effective mass:

$$\tau_{al} = \frac{\hbar^3 \rho U_l^2}{8\pi^2 k T E_1^2} \frac{1}{m^* k} \quad (\text{MKS}) \quad 4.22$$

For a parabolic band, the equation $\hbar^2 k^2 / 2m^*$ applies; substituting k in equation 4.22:

$$\tau_{al} = \frac{\hbar^4 \rho U_l^2}{8\pi^3 k T E_1^2 (2m^*)^{3/2} E^{1/2}} \quad (\text{MKS}) \quad 4.23$$

For a non-parabolic band, using equation 4.5 and substituting m^* in equation 4.22:

$$\tau_{al} = \frac{\hbar \rho U_l^2}{2k T E_1^2} \frac{1}{k^2} \frac{dE}{dk} \quad (\text{MKS}) \quad 4.24$$

Note that this can be written in the form:

$$\tau_{al} = (\tau_o)_{al} k^{2s-1} \frac{dE}{dk} \quad 4.25$$

where s is equal to $-\frac{1}{2}$ and is defined as the scattering parameter.

The form of equation 4.25 will be shown to apply to many scattering mechanisms and could be called "the generalized form" of the scattering laws in the case of spherical constant energy surfaces and non-parabolic bands.

The constant τ_o will be seen to be a function of the temperature only.

For ellipsoidal constant energy surfaces, it was shown by Herring and Vogt (56H1) that E_1 is related to Ξ_d and Ξ_u deformation potential constants which depend on the symmetry of the valleys considered. The effective mass to use in this case would be the density of states effective mass, equation 4.18.

4.4.2. Acoustic phonon scattering, piezoelectric.

This type of scattering is due, as in the previous case, to the acoustic mode of vibration except that a phase difference of 90° exists between the matrix elements of each case. It is only possible in crystals lacking a center of symmetry. Using a model of a layered lattice, Arlt and Quadflieg (68A2) show that three mechanisms may contribute to the piezoelectric effect: the internal displacement of the

ionic charge, of the electronic charge and the change in ionicity due to strain.

Harrison (56H2) determined the relaxation time for electron scattering. The results are:

$$\tau_{pi} = \frac{\rho U_l^2 h^3 \kappa_o^2}{8\pi^4 e^2 kT \alpha C} \frac{k}{m} \quad 4.26$$

C : measured piezoelectric constant.

α : a constant which depends on the crystallographic direction.

κ_o : static dielectric constant.

If m is replaced by the effective mass, then in the case of a non-parabolic band:

$$\tau_{pi} = \frac{\rho U_l^2 h^3 \kappa_o^2}{2\pi^2 e^2 kT \alpha C} \frac{dE}{dk} \quad 4.27$$

If equation 4.27 is written in the generalized form, it is seen that the scattering parameter will be $s = +\frac{1}{2}$ for this case.

4.4.3. Intraband optical phonon scattering

The optical branch of the lattice vibrations is now thought to be the important one in III-V compounds (57E1, 60E1). Rode (70R1, 71R1) corroborates this conclusion.

At high temperatures where $kT \gg h\nu_o$, ν_o being the frequency of the longitudinal mode of the optical branch, the collisions are elastic and Howarth and Sondheimer (53H1) have derived a time of relaxation for the case of a single energy band. They found (p. 59, 53H1):

$$\tau_{po} = \frac{a^3 M h \nu_o^2}{2 e^4 kT} \frac{dE}{dk} \quad 4.28$$

where "a" is the interionic distance and M is the reduced mass of the ions. The scattering parameter is therefore as in the case of piezoelectric scattering, $s = + \frac{1}{2}$.

When optical phonon scattering is present in a material, the mobility of carriers can be calculated either by the relaxation time method or using variational methods. When the scattering mechanism is elastic, a relaxation time characterizing the rate at which momentum decays can be defined. From the relaxation time, one can calculate the perturbation of an equilibrium electron distribution by a small electric field and, hence the mobility. When the scattering is inelastic, no relaxation time exists exactly, although in certain limits this approximation can be useful.

Of all the electron scattering mechanisms mentioned in this work, only optical phonon scattering is an inelastic process. In the work of Rode (70R1) mentioned above, the drift mobility is calculated by a simple iterative technique of solution which he claims, retains all the advantages of variational techniques without, however, the need for excessive mathematical detail. The first iteration in his procedure

gives the usual result for a relaxation time approximation; he also quotes that for GaAs, at 300°K, the use of only the first iteration leads to an underestimate of the true mobility by 33%.

Ehrenreich (61E1) found that the value of s falls from $+\frac{1}{2}$, at high temperatures, to a value of zero as the temperature decreases and approaches $T = \hbar \nu_0 / k$; this temperature is called the critical temperature. Values of this critical temperature are reproduced in Table 4.1 for several III-V compounds (64M1).

TABLE 4.1

Critical temperatures for some III-V compounds.

InSb	264°K	GaSb	336°K
InAs	334	GaAs	408
InP	487	AlSb	482
		GaP	578

Although these considerations show that at lower temperatures the relaxation time method is not strictly valid, many authors have still made use of this method when the resulting inaccuracies are not too large. Here, this convention will be followed and throughout the analysis, the optical phonon scattering will be represented by a convenient relaxation time. However, care will be taken to note the possible errors resulting from this approximation.

For the case of a non-parabolic band, Conwell and Vassell (68C1) have derived the following expression for optical phonon scattering:

$$\frac{1}{\tau_{po}} = eE_o (2N_{ql} + 1) (2m_o^* \gamma)^{-1/2} \frac{d\gamma}{dE} \quad (\text{MKS}) \quad 4.29$$

where

$$eE_o = \frac{e^2 m_o^* \hbar \omega_l}{4\pi \hbar^2 \epsilon_o} \left(\frac{1}{\kappa_\infty} - \frac{1}{\kappa_o} \right) \quad (\text{MKS}) \quad 4.30$$

$$N_{ql} = \frac{1}{(e^{\hbar \omega_l / kT} - 1)} \quad (\text{MKS}) \quad 4.31$$

and

$$\gamma = \frac{\hbar^2 k^2}{2m_o^*} \quad (\text{MKS}) \quad 4.32$$

With

$\hbar \omega_l = \hbar \nu_o \equiv$ longitudinal optical phonon energy.

$E_o \equiv$ effective electric field that determines the strength of electron coupling to the polar modes.

$N_{ql} \equiv$ number of lattice quanta in the lattice mode considered.

$\kappa_\infty \equiv$ high frequency dielectric constant.

$\epsilon_o \equiv$ permittivity of free space = $8.85 \times 10^{-12} \frac{\text{coul.}^2}{\text{N.m}^2}$.

It is pointed out by Conwell and Vassell (68C1) that the expression for τ_{po} was derived assuming only wave functions with s symmetry. Neglecting

the admixture of p functions causes the expression to be less accurate for higher energies. This is discussed in Zawadzki and Szymanska (7121) and it will be taken up later in the discussions.

4.4.4. Interband optical phonon scattering

In semiconductors with a band structure such that two bands have minima, which are close in energy, the scattering of carriers between the two bands may be important in determining the mobility of carriers in either one or both bands.

In polar semiconductors, interband scattering is possible if a carrier absorbs or emits an optical phonon, since a large change in wave vector k is necessarily required when the two minima are at different symmetry points in the Brillouin zone.

An expression for this type of scattering was derived by Conwell and Vassell (68C1) and the relaxation time is given by:

$$\frac{1}{\tau_{ib}} = \frac{D_{12}^2 (M_d^*)^{3/2}}{\sqrt{2} \pi \hbar^3 \rho \omega_{12}} \cdot \frac{1}{e^{x_{12}} - 1} \cdot \left[(E + \hbar\omega_{12} - E_{12})^{1/2} + e^{x_{12}} (E - \hbar\omega_{12} - E_{12})^{1/2} \right] \quad 4.33$$

(MKS)

where D_{12} is the coupling constant, ω_{12} the angular frequency for transition between the two bands, $x_{12} = \hbar\omega_{12}/kT$, E_{12} is the energy

separation of the two minima and $M_d^* = M^{2/3} m_d^*$. The integer M represents the number of equivalent minima.

Note that this type of scattering is subjected to the same limitations as with the intraband optical phonon case.

If equation 4.33 could be reduced to the "generalized form", considering the general shape of the curve of τ versus E for this scattering mechanism, the value of the scattering parameter s would probably be negative.

4.4.5. Ionized impurity scattering

The problem of ionized impurity scattering was originally treated by Conwell and Weisskopf (50C1). The divergence difficulty arising from Rutherford scattering was corrected by Brooks and Herring (51B1) and Dingle (55D1) who used a screened Coulomb potential. This approach lead the way to a relaxation time expressed as (59S1):

$$\tau_I = \frac{16\pi (2m^*)^{1/2} (\epsilon_o \kappa_o)^2 E^{3/2}}{Z'^2 e^4 N_I f(Z)} \quad (\text{MKS}) \quad 4.34$$

where Z' is the charge of the ions and $f(Z)$ is a slowly varying function of E and is given by:

$$f(Z) = \ln(1 + Z) - \frac{Z}{1 + Z} \quad 4.35$$

with $Z \equiv (2ka)^2$ and "a" is the screening distance which is a function of the carrier density, temperature and energy of the carrier.

The above screening relation was derived by a quantum-mechanical treatment and is based on the Born approximation, which implies that the range of validity of the treatment is given by $Z \gg 1$. When this is violated as in the case of high impurity concentration or at very low temperatures, the accuracy of the calculation may be compromised.

Using the results of Dingle (55D1) and Beer (63B1), a relation for Z is obtained in the form.

$$Z = \frac{8\epsilon_o \kappa_o m^* kT E}{e \hbar^2 n} \frac{F_{1/2}(\zeta)}{F_{-1/2}(\zeta)} \quad (\text{MKS}) \quad 4.36$$

where n is the carrier concentration in the conduction band and the F 's are Fermi integrals defined as usual:

$$F_r(\zeta) = \int_0^\infty \frac{x^r dx}{1 + e^{x-\zeta}} \quad 4.37$$

The above theory for parabolic bands has been extended by Ehrenreich and Moore (66E1) and later by Moore (67M1), to include quantum-mechanical corrections to the semi-classical Brooks-Herring treatment. The following expression for the mobility is derived:

$$\mu_I = \mu_I^* \{1 + \sigma_B + \sigma_M + \sigma_D\} \quad 4.38$$

where μ_I^* is the Brooks-Herring mobility and the correction terms σ_B , σ_M and σ_D are defined by Ehrenreich and Moore (66E1). The integrals involved have been solved numerically by Moore (67M1) for the case of GaAs.

When the non-parabolicity is taken into consideration, Kolodziejczak (61K2), calculated the value of the screening distance "a". The relaxation time may be written as (Barrie (56B1)):

$$\tau_I = \frac{8\pi \hbar^2 \epsilon_o^2 \kappa_o^2 k^2}{e N_I f(Z)} \frac{dE}{dk} \quad (\text{MKS}) \quad 4.39$$

where Z is still given by $(2ka)^2$, but (61K2),

$$a^2 = \frac{2\pi^2 \epsilon_o \kappa_o \hbar^3}{e^2 (2m_o^*)^{3/2} (kT)^{1/2}} \frac{1}{L_1^{1/2}(\beta, \zeta)} \quad (\text{MKS}) \quad 4.40$$

Here, $L_1^{1/2}(\beta, \zeta)$ is an integral defined as:

$$L_a^b(\beta, \zeta) = \int_0^\infty \left(-\frac{df_o}{dx} \right) (x + \beta x^2)^b (1 + 2\beta x)^a dx \quad 4.41$$

where $\beta = \frac{\hbar^2 T}{E_o^*}$ and ζ is the reduced Fermi energy.

However, if we have multiple charged scattering centers and carriers present in more than one band, Kolodziejczak relations 4.40 and 4.41 have to be modified to take this into account. Baxter et al. (67B1) have shown that this can be done by replacing N_I in equation 4.39 by $\sum_i Q_i^2 N_i$, where Q_i and N_i are the charge and density of the i^{th} scattering center respectively. They have also shown that in order to take into account the difference of screening by the carriers in the different bands, the screening distance "a" must be replaced by the one given by

Dingle (55D1):

$$\frac{1}{a^2} = \frac{e^2}{\epsilon \kappa_o kT} \sum_i \frac{\partial n_i}{\partial \zeta} \quad (\text{MKS}) \quad 4.42$$

where n_i is the density of carriers in band i . (Appendix 4.1 shows how $\partial n_i / \partial \zeta$ can be calculated).

Looking back at equation 4.39, the scattering parameter s will be found to be equal to $+\frac{3}{2}$.

4.4.6. Space-charge scattering

This scattering mechanism was first observed by Weisberg and Blanc (60W1) in GaAs. It is usually called the anomalous scattering mechanism or "mobility killer" because it reduces the total mobility. It is based on a model of space-charge regions devised by Crawford and Cleland (59C1) and Gossick (59G1) to explain lowered mobilities in neutron-irradiated germanium. These space-charge regions are formed by randomly distributed acceptor impurities, compensating the donors (large disordered regions of modified conductivity type) which would tend to produce intrinsic or even p-type regions. These regions would be surrounded by space-charge which could be much larger in size than the disordered regions themselves.

It could also be expected that these potential variations could result from fluctuations in the concentration of a deep acceptor-

level impurity; for example, oxygen doping in GaAs (66K2) reduces the mobility.

This space-charge scattering mechanism has, up to now, been included in several studies of GaAs and GaP. By assuming that these regions are impenetrable spheres to the quasi free electrons, Conwell and Vassell (68C1) have obtained an expression for the relaxation time due to this mechanism. For non-parabolic bands and spherical energy surfaces, it is stated as:

$$\tau_{sc} = (N_s Q_s)^{-1} (m_o^*/2\gamma)^{1/2} d\gamma/dE \quad 4.43$$

where N_s is the density of the impenetrable spheres and Q_s is the scattering cross-section.

From equation 4.43, the scattering parameter s would have a value of $-\frac{1}{2}$ in the generalized form equation for τ . A recent paper by Hamerly and Heller (71H1) on n-GaAs includes space-charge scattering in their study. Their experimental results indicate that this situation can dominate at room temperature in highly compensated n-GaAs. They also suggest a slightly stronger energy dependence of τ on energy, their results indicating a value for s equal to $-\frac{5}{6}$.

It is obvious that the exact energy dependence of the relaxation time is not yet well established. Thus, incorporation of τ_{sc} into the calculations can only be considered as an imperfect attempt to take this mechanism into account.

4.4.7. Alloy scattering

It is expected that in disordered alloys, there will be a contribution to the scattering of carriers from the randomly positioned perturbations of the lattice by the alloy atoms. This can be discussed, at least in a qualitative manner, from a perturbation approach suggested by Nordheim (31N1) and also used by Brooks (unpublished) with an added assumption about the magnitude of the perturbation.

Nordheim's results, as quoted by Glicksman (58G1) are:

$$\frac{1}{\tau_{\text{all}}} = \frac{8\pi^3}{h^4} (UV) (2m_L m_T)^{1/2} E^{1/2} x (1-x) \quad 4.44$$

where U is an integral over scattering angles of the square of the matrix element for the difference of the potentials of the two components of the alloy, V is the atomic volume, x is the mole fraction of the minority component in the alloy and m_L , m_T are the electron longitudinal and transverse effective masses.

The unknown U has been suggested by Brooks to represent the difference in potential between the conduction band edges of the unalloyed components.

Tietjen and Weisberg (65T1) give the theoretical expression for the mobility due to alloy scattering as:

$$\mu_{\text{all}} = \frac{(2\pi)^{1/2} e \hbar^4 N_a}{3 (kT)^{1/2} m^{*5/2} (E_1 - E_2)^2 x (1-x)} \quad 4.45$$

where N_a is the density of lattice sites equal to $1/V \text{ cm}^{-3}$ and $(E_1 - E_2)$ is the energy separation between the conduction band edges of the unalloyed components.

Equation 4.45 can be expressed as:

$$\mu_{\text{all}} = \text{constant} / (m^*/m)^{5/2} (E_1 - E_2)^2 x(1-x) \quad 4.46$$

Since equations 4.45 and 4.46 are in an integrated form, the present author used a relaxation time dependent on energy, of the form:

$$\frac{1}{\tau_{\text{all}}} = \frac{8\pi^3}{h^4} (E_1 - E_2)^2 \frac{1}{N_a} 2^{1/2} m^{3/2} E^{1/2} x(1-x) \quad 4.47$$

$$\frac{1}{\tau_{\text{all}}} = \text{constant } E^{1/2} \quad 4.48$$

where the "constant" could be written as:

$$\text{constant} = C \left[\frac{8\pi^3}{h^4} (E_1 - E_2)^2 \frac{1}{N_a} 2^{1/2} m^{3/2} x(1-x) \right] \quad 4.49$$

where C is a factor which will account for any correction necessary in the theory.

Equation 4.48 can be shown to have a scattering parameter

$$s = -\frac{1}{2}$$

4.4.8. Other scattering mechanisms

Various other scattering mechanisms such as neutral impurity scattering (50E1), dislocation scattering (54R1) and electron-electron scattering (59S1) can be shown to be negligible in the compounds studied, under the experimental conditions involved here.

4.4.9. Summary

Most of the scattering mechanisms described, have been shown to obey a scattering law, which could be reduced to a general form.

This form of τ has been suggested initially by Zawadzki (62Z1) and is used extensively in transport properties of semiconductors.

The equation

$$\tau_i = (\tau_o)_i k^{2s_i-1} \frac{dE}{dk} \quad 4.50$$

is seen to vary with energy E and wave vector of the electrons k . $(\tau_o)_i$ is a constant for one type of scattering and includes all the parameters which are independent of E and k .

Each value of s_i represents the individual scattering mechanisms. However, this form of equation will be applied to the experimental results and if more than one scattering mechanism is present, the effective s determined will be somewhere between these

separate s values.

For a parabolic band, equation 4.50 reduces to:

$$\tau_i = c_i E_i^{s_i} \quad 4.51$$

Table 4.2 summarizes these results for the possible values of s .

TABLE 4.2

Value of the scattering parameter s for each scattering mechanism

obeying the relation $\tau_i = (\tau_o)_i k^{2s_i-1} \frac{dE}{dk}$.

scattering mechanism	s_i
Ionized impurity	+ 3/2
Acoustic, piezoelectric	+ 1/2
Intraband optical phonon	+ 1/2
Interband optical phonon	(negative)
Acoustic, "deformation potential"	- 1/2
Space-charge	-1/2(-5/6)
Alloy	- 1/2

CHAPTER 5

EXPERIMENTAL

5.1. SAMPLES AND PREPARATION

The alloy system of $\text{Ga}_{1-x}\text{In}_x\text{As}$ was prepared in this laboratory by a former graduate student of our group, Dr. W. Coderre. The horizontal Bridgman or step-freeze technique was used (69C1). The resulting ingot was about 15 cm long and 1 cm wide, the cross-section being elliptical. It was polycrystalline, the composition varying smoothly along the length up to approximately $x = 0.75$. Slices were cut from the ingot and the composition was found by determining the lattice parameter from X-ray powder photographs. The lattice parameter a_0 was then compared with a curve of a_0 versus x (58W1).

The samples were prepared from the cross-sectional slices in the form of parallelepipeds of dimensions 10 x 3 x 1 mm. For the measurements of the transverse N.-E. coefficient, the geometry of the sample had to be perfect; otherwise the sample would not remain in the sample holder.

Good measurements for the Hall coefficient (constant thickness), resistivity (rectangular cross-section) and transverse N.-E. coefficient (length, width) depend on the accuracy with which the dimensions can be measured. Thus, a careful lapping was done using the

available equipment in our laboratory and the geometry of the major face was checked to be rectangular. The dimensions were measured with a micrometer accurate to one micron.

The GaSb sample was provided by J. Basinski of the semiconductor group. Transport measurements had already been made in this laboratory and different parameters were available. The magneto-Seebeck and transverse N.-E. effects were both measured on that specimen.

5.2. ELECTRICAL CONTACTS TO THE SAMPLES

The magneto-Seebeck effect was measured on twelve samples; it will be seen in the description of the apparatus that only pressure contacts on the specimens were needed.

The Hall effect measurements, made on all the samples, required two current contacts at the ends and two Hall contacts on opposite sides. They consisted of small diameter gold wires, spark welded to the specimen by discharging through the contacts a variable capacitor (1-20 μ f) charged to a variable voltage, 1-30 volts. The capacitor was discharged in both directions until ohmic contacts of approximately 1-5 ohms were obtained. The carrier concentrations determined from those measurements ranged from 1.12×10^{16} to $7.02 \times 10^{17}/\text{cm}^3$.

The transverse N.-E. effect was observed on InAs and on four samples of the alloy system. Two opposite contacts were spark welded on the sides in a similar way. The size of the wires for the

transverse N.-E. effect is very critical. The contacts were made to the sides with very small diameter (0.003") gold wires. This is necessary so, as not to short-circuit the thermoelectric power; this would automatically lead to an overestimation of the transverse N.-E. effect.

Mochan and Smirnova (60M1) made measurements of the transverse N.-E. effect on p-type germanium. The side contacts were tin dots of diameter 1.0 mm. They found that the value of Q_1 decreased as the dimensions of the dots were decreased. Their explanation is the following: that part of the germanium which was shorted by the tin dots acted like a short-circuited thermoelement; this caused a positive charge to appear at the cold end of the dot. When the magnetic field is turned on, in addition to the transverse N.-E. potential difference, one can expect a Hall effect to appear; it is caused by circulating currents in the vicinity of the electrodes which give rise to an additional positive potential difference. The observed effect always had a positive sign even for n-type germanium.

The size of the contacts made in this case is of the order of 0.08 mm so as to avoid this type of situation. The ideal situation is to have a sample in the form of a cross.

Resistivity measurements were necessary on the same five samples. Electroplating was used to produce a thin film of indium on the two ends and on two narrow strips on one side of the specimen. The indium was annealed for a short period of time in an inert gas, thus producing ohmic contacts.

5.3. APPARATUS AND DETAILS OF SAMPLE THERMAL CONNECTIONS

The Hall coefficient measurement, being now a very standard means of calculating the carrier concentration, will not be described here. The following description applies only to the thermal measurements.

When the author started this program of research, an apparatus had been designed and built by Dr. M. Aubin, now at Sherbrooke University. He had made magneto-Seebeck effect measurements on the system of alloys of $\text{InAs}_x\text{Sb}_{1-x}$ and $\text{GaIn}_x\text{Sb}_{1-x}$.

The present author made a complete set of measurements on the system of $\text{GaIn}_x\text{As}_{1-x}$ of the magneto-Seebeck effect using the same apparatus. The sample holder, the sink and the heater are shown in figure 5.1 (As of (69A2), figure 3.6). The specimen was held in a horizontal position and contact with it was made through two insulated copper rods which were lowered onto it.

This apparatus will not be described any further because it was not adequate to measure the transverse N.-E. effect. The length along which the thermal gradient was applied could not obviously be estimated and this was needed to calculate the transverse N.-E. coefficient. Another system was therefore designed and built to serve this purpose. Figure 5.2 gives a view of the "ensemble" of the experimental set-up with a simplified circuit diagram in a block diagram form.

The sample holder itself is shown in details in figure 5.3. It is made completely out of non-magnetic materials and the thickness is

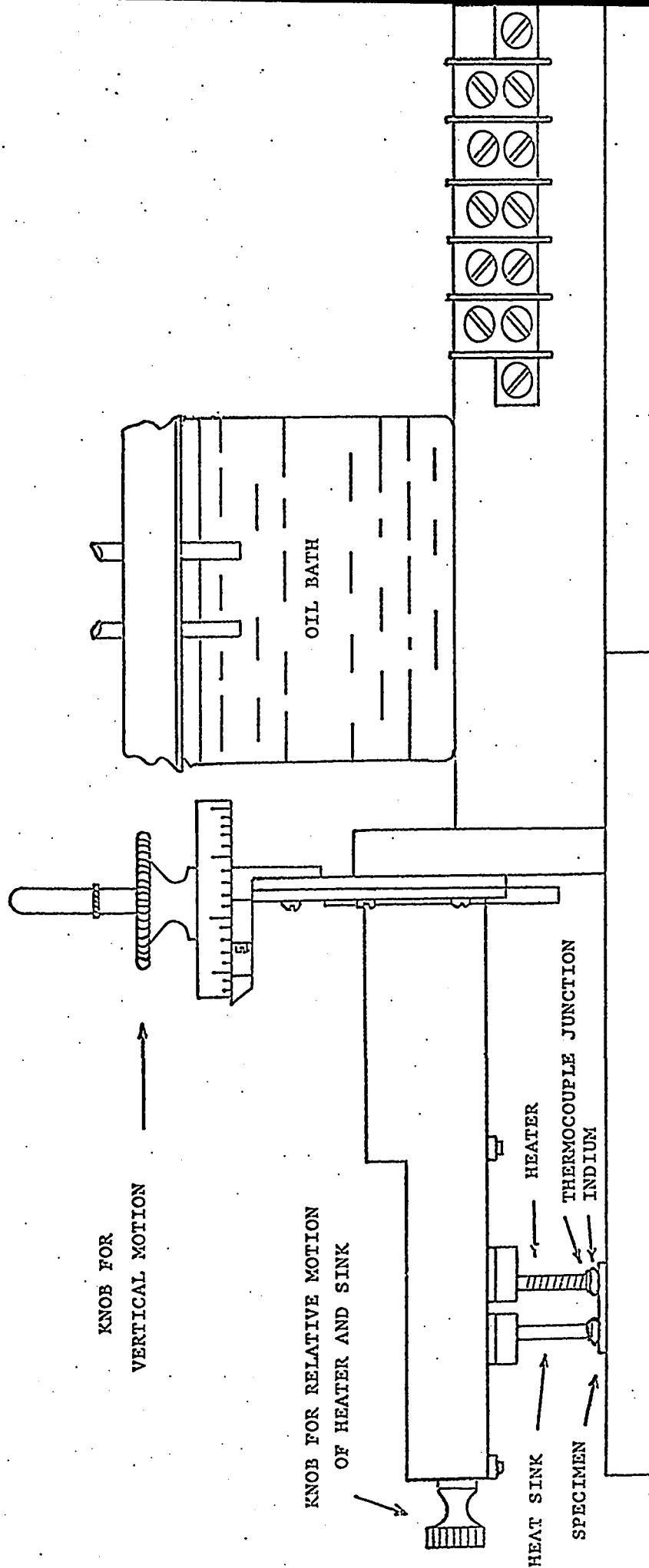


Figure 5.1 Initial magnetothermoelectric power apparatus

minimized so as to fit in between the magnet poles. The heater and the sink are applied to the ends of the sample with the junctions of the copper-constantan strip thermocouple being inserted at each end. One strip, at the sink end, acted as the cold junction and the other at the heater end being the hot junction.

Both the heater and the sink are electrically insulated, the support being made out of perspex. The sink represents a total mass of 30 grams of copper.

A good thermal contact of the thermocouple strips with the specimen is assured by inserting thin sheets of indium at the three points shown on the figures and by applying a relatively high pressure on the sample using the screw adjustment at the sink end, figure 5.3.

Since the temperature is measured by a differential method, a thin piece of sapphire (294 μ) is used to provide the electric insulation but still a very good thermal conduction.

A temperature difference of approximately 2 degrees was maintained between the ends of the sample by applying a regulated D.C. voltage to the heater wire with a Harrison Laboratories Constant Voltage supply, model 6343A.

A selection switch (figure 5.2), a twelve position double deck switch with silver contacts to minimize the electrical noise, provided the following readings:

Position 1.

Voltage difference produced by the thermocouple strip junctions; the temperature difference could then be calculated.

Position 2.

Voltage along the sample produced by the thermal gradient and the changes in voltage produced by the applied magnetic field.

Position 3.

Transverse N.-E. voltage produced by the magnetic field.

The selection switch sent the signal to a preamplifier, an Astrodata Nanovolt Amplifier, model 120, whose noise level was less than 0.05 μ V. Ten scales offered fixed gains varying from 200 to one million. The voltage was read on a four figure digital voltmeter (and also a six figure DANA, model 5330).

The Nanovolt amplifier was equipped with a potentiometer so that the voltage as read on the voltmeter could be nulled; this was useful to measure small changes in voltage.

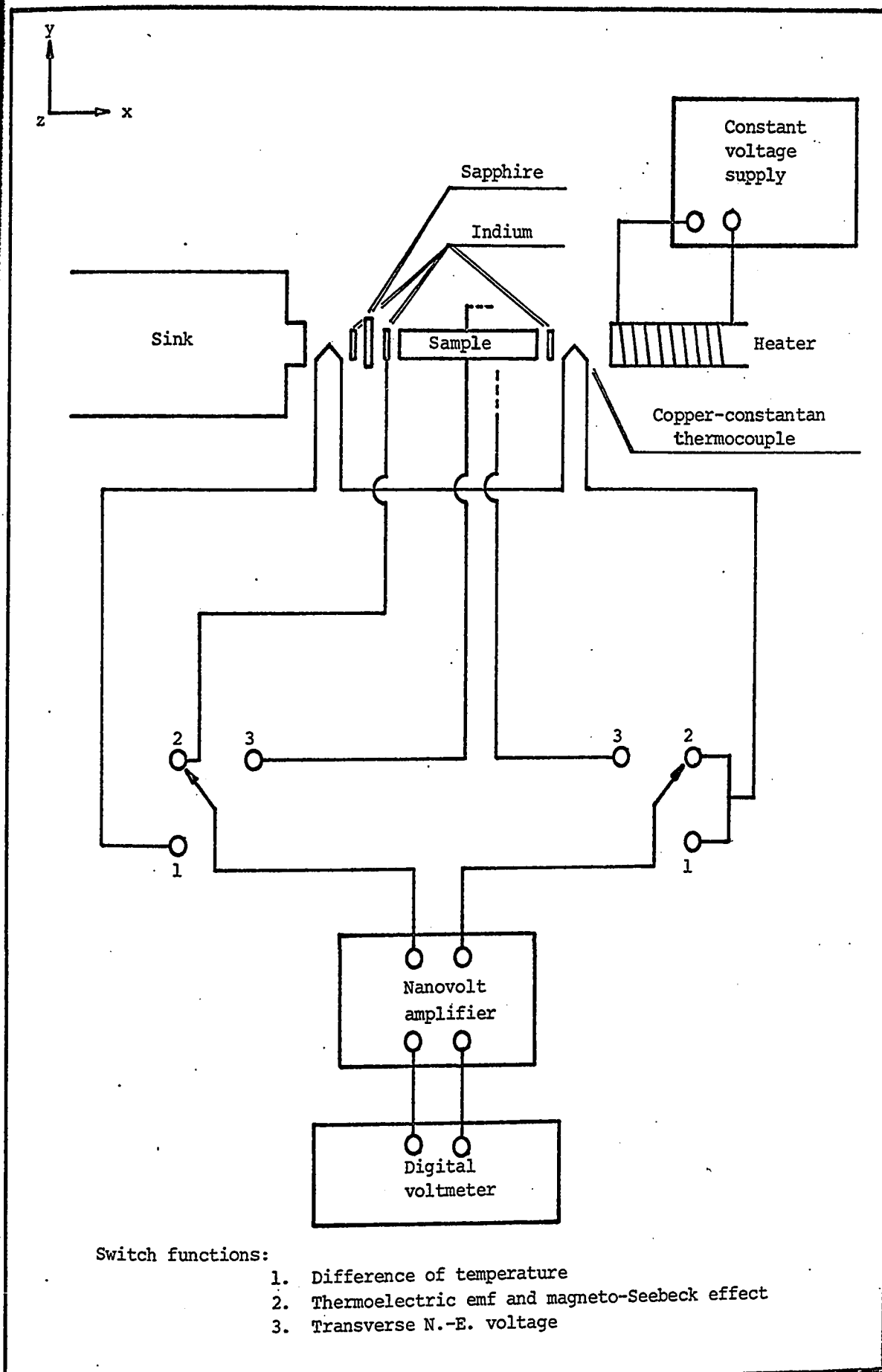


Figure 5.2 Electrical circuit for the magneto-Seebeck and transverse N.-E. effects

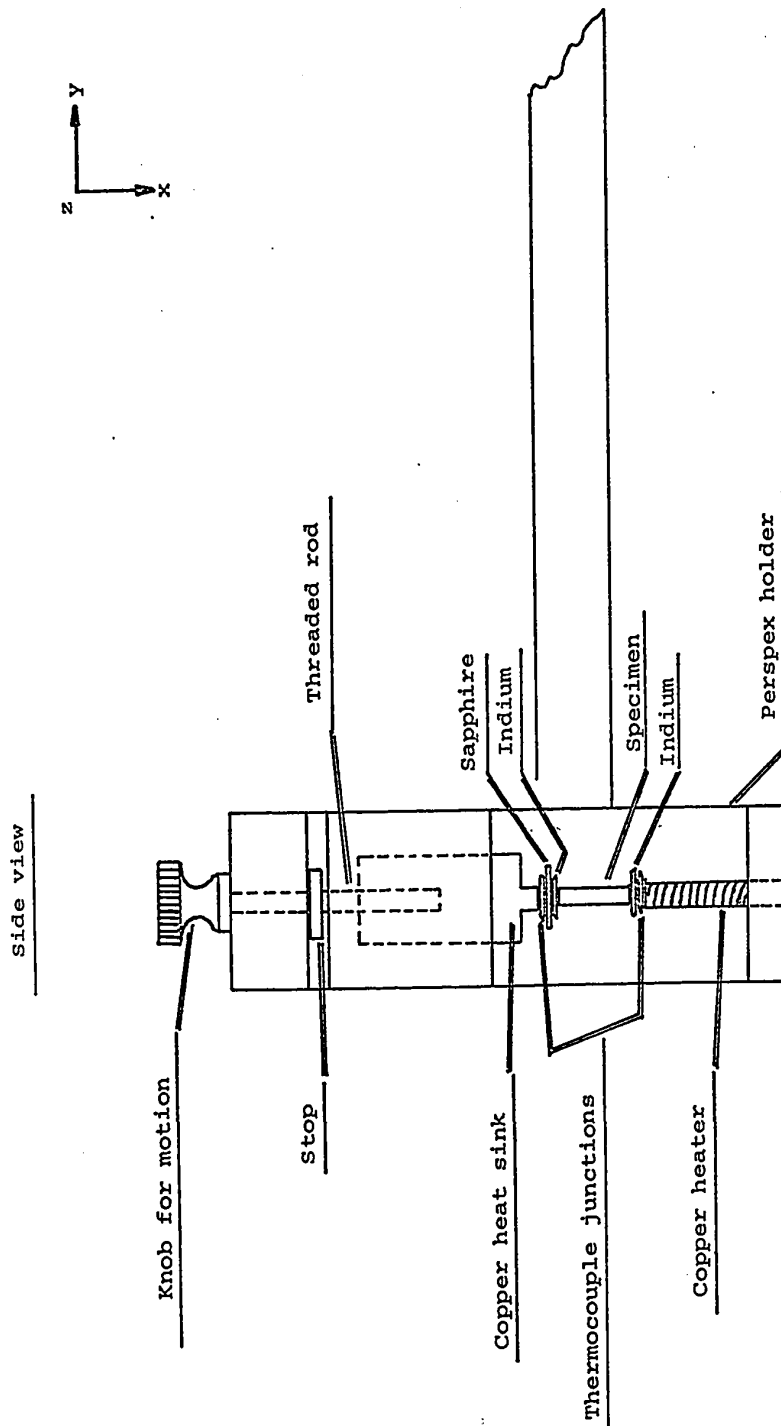


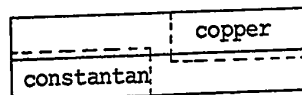
Figure 5.3 Sample holder

5.4. COMMENTS

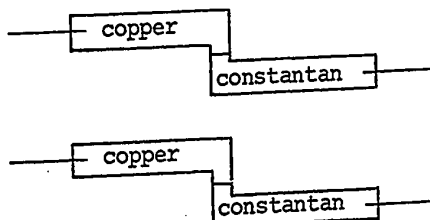
5.4.1. Measurement of the thermal gradient

Measuring the difference of temperature using an absolute method, that is, with separate cold junctions for each thermocouple immersed in an oil bath at a known temperature, so that the temperature of each end of the specimen can be determined independently and then the difference found, does not provide with more accuracy. This method had been used by Dr. M. Aubin on the original apparatus and his conclusions were that the noise plus the addition of the absolute errors in the subtraction made the differential method as accurate.

The copper-constantan ribbon was cut as shown below to form a small junction.



The voltage was measured across the 2 copper wires and a constantan wire joined the constantan strips of each junction.



The 4 contact wires were spot-welded to avoid any other junctions.

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This half and half copper-constantan ribbon had been available from the National Research Council of Canada and the calibration was provided to be $41.5 \mu\text{V}/\text{degree}$ at room temperature.

5.4.2. Thermal contacts

It is interesting to note that this apparatus will measure a temperature gradient larger than the one existing along the sample because of the presence of sapphire and indium sheets; this means that the thermoelectric power will always be lower than the true one.

The objective is therefore to obtain as high as possible a value for the thermoelectric power by minimizing the thicknesses of the sapphire and of the indium sheets. For a sample of length 10 mm, the extra thickness is about 300μ ; this represents, assuming for the indium and the sapphire, a thermal conductivity like that of the sample, a thermoelectric power 3% too low. Considering that the sapphire and indium sheets are highly conductive, this 3% value is reduced considerably. If mica of thickness $3-5 \mu$ is used instead of sapphire, the thermoelectric power goes down by a few percent.

A second systematic error which has to be mentioned although small, is that the size of all the wires coming into contact with the thermal flux should be minimized to avoid heat leakage.

5.4.3. Survey of the experimental error

The author takes it as being very important to mention that the described apparatus and crystal support gave very good results considering that any thermal measurement is not easy to perform.

When the magneto-Seebeck effect was measured with the original apparatus, a correction or calibration factor of 5% had to be applied to the infinite magnetic field value of the thermoelectric power in order to obtain the correct value for the effective mass, InSb being used as a standard. The apparatus described herein, gave good values of effective masses without having to use any correction factor. All the results described in this thesis are therefore those as obtained from the measurements.

Concerning those measurements, it is not easy to calculate the experimental error, the largest source of error and the most difficult to estimate being an imperfect thermal contact between the specimen and the thermocouple.

Other sources of errors are the measurement of the emf with the digital voltmeter, the thermoelectric power of the passive element with reference to which the specimens are measured and the error in the calibration of the thermocouple.

5.5. MAGNETIC FIELD

The measurements were performed with a Magnion-Harvey-Wells 15 inch electromagnet Model L-158 along with the HS-10200 Power Supply and FFC-4 Field regulator. With a gap of $1\frac{1}{4}$ " and a maximum current of 205 amperes, a field of 3.20 Wb/m^2 is obtained. The technical details can be found in the company manual; let us say that the field set accuracy is 5 parts in 10^5 and the stability 1 part in 10^6 .

The sample holder was placed in the center of the pole gap where the field is constant to 1 part in 10^5 over a cubic centimeter. The gaussmeter probe has to be moved to an outside position to make way for the sample holders or cryostats. A calibration curve is available in the laboratory relating the value of the magnetic field indicated by the dials of the magnet and the real field at the center of the pole gap.

5.6. MEASUREMENT PROCEDURE

It was a very delicate operation to install the sample in the holder with the sapphire and the indium sheets. Once that was done and the sample staid in position under the applied pressure, the electrical side contacts were made with the gold wires.

The sample holder was then insulated from the room so that the measurements would not be affected by air currents, etc, and it was adjusted in between the magnet poles.

A period of two hours or more was usually necessary until the system reached thermal equilibrium. During that process, the pressure was increased to improve the thermal contacts. The thermoelectric power was observed until a stable reading was reached.

This process was repeated two or three times for each sample until a value of the maximum thermoelectric power could be estimated.

When the system showed good thermal contacts, that is, a high value of the thermoelectric power, the magneto-Seebeck and the transverse N.-E. effects were measured.

The magneto-Seebeck effect is an even function of the magnetic field; therefore, the voltages read with the field in both the normal and reversed directions were simply averaged out.

The transverse N.-E. effect is an odd function of the field. The corresponding voltage is:

$$V_{yl} = V_N + V_{R.L.} + V_T \quad 5.1$$

with the field in one direction

- V_N : Transverse N.-E. voltage
- $V_{R.L.}$: Righi-Leduc voltage
- V_T : Voltage produced by the off-set of the probes
with respect to one another.

If the field is reversed and a quick measurement is made, the Righi-Leduc voltage does not have time to reverse its direction, (65E1):

$$V_{y2} = -V_N + V_{R.L.} + V_T \quad 5.2$$

Subtracting these two equations:

$$V_N = \frac{1}{2} (V_{y1} - V_{y2}) \quad 5.3$$

which is to be substituted for V_y in equation 2.6.

This procedure was followed and it was useful to eliminate V_T . The Righi-Leduc voltage can be eliminated this way for weak magnetic field values where the field can be reversed quickly.

Temperature gradients cannot follow an order of 50 cycles per second; the field needs to be reversed and the measurement made within 1/100th of a second. This is impossible with the equipment available in our laboratory. However, as will be shown later, the Righi-Leduc effect is small in semiconductors having a large phonon thermal conductivity; it was therefore neglected.

It was mentioned in chapter 2 that the thermomagnetic effects can be either adiabatic or isothermal effects. It is experimentally convenient to measure the adiabatic thermomagnetic coefficients but the adiabatic formulae are more complex. However, the isothermal coefficients can be simply expressed in terms of the adiabatic coefficients as:

$$\alpha_i = \frac{\alpha_a + B^2 (Q_1)_a S}{1 + B^2 S^2} \quad 5.4$$

and

$$(Q_L)_i = \frac{(Q_L)_a - \alpha_a S}{1 + B S^2} \quad 5.5$$

These equations follow from Heurlinger relations (p. 79, 67H1), where the subscripts "a" and "i" signify adiabatic and isothermal respectively.

Usually the adiabatic values are measured and the isothermal values are found using these expressions. If, however, the Righi-Leduc coefficient S is small or zero, equations 5.4 and 5.5 reduce to:

$$\alpha_i = \alpha_a \quad 5.6$$

and

$$(Q_L)_i = (Q_L)_a \quad 5.7$$

Indeed, the coefficient S is very small in semiconductors. Smith (p. 187, 59S1) calculates its value for a typical semiconductor with $\alpha_a = -500 \mu V/^{\circ}K$. When the transverse N.-E. voltage is $1 \mu V$, the Righi-Leduc voltage is $10^{-4} \mu V$. These voltages give the following values:

$$S = 2 \times 10^{-6} m^2/volt.sec$$

$$(Q_L)_a = 10^{-5} m^2/sec. ^{\circ}K$$

This example, no doubt, gives validity to equations 5.6 and 5.7. They will be assumed in this work.

CHAPTER 6

GALLIUM INDIUM ARSENIDE

6.1. INTRODUCTION

In the case of the III-V compounds, it is now well established that of all the possible scattering mechanisms mentioned in chapter 4, optical phonon scattering is the important scattering mechanism. This, by interpolation, would be the mechanism to choose for the alloys also. This will be investigated.

However, it has been suggested by Tietjen and Weisberg (65T1) that alloy scattering has a negligible effect in the alloys except in the case of the $\text{Ga}_{1-x}\text{In}_x\text{As}$ alloy system where the effect would be the largest. It could account at high values of x , near $x = 0.60$, for up to 40% of the total scattering. Hockings et al (66H1) indicate a negligible or possibly minor amount of alloy scattering in n-type specimens because the mobilities are high. All the results for the III-V alloys, $\text{InAs}_{1-x}\text{P}_x$, $\text{Ga}_{1-x}\text{In}_x\text{Sb}$, $\text{Al}_{1-x}\text{In}_x\text{Sb}$ and $\text{GaP}_{1-x}\text{As}_x$, are in marked contrast to the $\text{Ge}_{1-x}\text{Si}_x$ alloys where the presence of alloy scattering is well established (64A1).

Because of the nature of alloy scattering, which could be described as a short range disorder causing an aperiodicity in the crystal potential, it is impossible to distinguish between this and the presence of inhomogeneities. Inhomogeneities as described by space-charge

scattering, if present, are distributed in the whole crystal and are more of a long range disorder type.

When the longitudinal and transverse N.-E. effects are measured under weak magnetic fields, both in the non-degenerate and strongly degenerate limits, the coefficients of both effects are proportional to the scattering index s . Therefore, for a single scattering mechanism, the sign of the effects distinguishes between various scattering mechanisms. For "deformation potential" scattering, alloy scattering and space-charge (inhomogeneities) scattering, $s = -\frac{1}{2}$, the effects should be positive; for polar optical and piezoelectric scattering, $s = +\frac{1}{2}$, they should be negative and for ionized impurity scattering, $s = +\frac{3}{2}$, they should have larger negative values.

Such measurements have been made on gallium arsenide (59E1) and indium arsenide (60E2). In both cases, the effects had a negative sign at low temperatures and at high temperatures ($>550^{\circ}\text{K}$) they became positive. The negative sign was interpreted as charged impurity scattering, optical phonons being neglected due to the fact that the ionic component of chemical bonding is small.

Rodot (60R1) was the first to recognize that such information could be obtained, not only from the effects in low fields, but also from the longitudinal effect at high fields. The transverse effect decreases to zero as the field increases.

Later, Kolodziejczak and Sosnowski (62K1) showed that the sign, of both effects in low fields, can change due to a pronounced

non-parabolicity of the band structure. Hence, one has to be very careful in interpreting results from such measurements.

Furthermore, the transverse N.-E. effect is known today to be very sensitive to the presence of certain types of inhomogeneities which are to be distinguished from space-charge scattering. Drichko and Mochan (66D1) and Agaev, Mosanov and Ismailov (68A3) have shown this to be true for InSb. Even the presence of submicroscopic inhomogeneities may affect the measurements.

In the present work, the magneto-Seebeck and N.-E. effects have been investigated at room temperature (298°K), in a magnetic field of induction up to 3.2 Wb/m^2 . In the alloys considered, at the InAs end (small x) this value corresponds to a strong magnetic field, $\mu B \gg 1$; near the GaAs end of the alloy, B is in the intermediate range, $\mu B \approx 1$.

6.2. THEORY AS APPLIED TO $\text{Ga}_{1-x}\text{In}_x\text{As}$

In the measurements on this alloy system, the carrier concentrations were found to be between $1.12 \times 10^{16}/\text{cm}^3$ and $7.02 \times 10^{17}/\text{cm}^3$. In both InAs and GaAs, the Γ_{1c} band is the main conduction band; the next higher bands are situated far enough so that they do not contribute to conduction. In GaAs, the X_{1c} band is the nearest to the Γ_{1c} band; it is situated at 0.38 eV above the bottom of the Γ_{1c} band (72B3). In pure InAs, the L_{1c} band is at 0.70 eV above the bottom of the central conduction band (68K1). The values quoted are at 4.2°K.

Therefore, one conduction band is considered, the electron charge being $-e$.

The general equation for the magneto-Seebeck effect, equation 4.1, reduces in such a case to:

$$\alpha(B) = \frac{\sigma_{11}^0 \theta_{11} + \sigma_{12}^0 \theta_{12} + E_F/eT (\sigma_{11}^2 + \sigma_{12}^2)}{(\sigma_{11}^2 + \sigma_{12}^2)} \quad 6.1$$

where the above tensors are:

$$\begin{aligned} \sigma_{11} &= - \frac{e}{3\pi^2} \left\langle \frac{\mu}{1 + B^2 \mu^2} \right\rangle \\ \sigma_{12} &= - \frac{eB}{3\pi^2} \left\langle \frac{\mu^2}{1 + B^2 \mu^2} \right\rangle \\ \theta_{11} &= \frac{k}{3\pi^2} \left\langle \frac{\xi \mu}{1 + B^2 \mu^2} \right\rangle \\ \theta_{12} &= \frac{kB}{3\pi^2} \left\langle \frac{\xi \mu^2}{1 + B^2 \mu^2} \right\rangle \end{aligned} \quad 6.2$$

Equations 4.6, 4.7 and 4.8 become respectively:

$$\alpha(0) = - \frac{k}{e} \left[\frac{\langle \xi \mu \rangle}{\langle \mu \rangle} - \zeta \right] \quad 6.3$$

$$\alpha(\infty) = - \frac{k}{e} \left[\frac{\langle \xi \rangle}{\langle 1 \rangle} - \zeta \right] \quad 6.4$$

and

$$n = \frac{1}{3\pi^2} \int_0^\infty \left(-\frac{\partial f_0}{\partial \xi} \right) k^3 d\xi \quad 6.5$$

with

$$\langle A \rangle = \int_0^\infty \left(-\frac{\partial f_0}{\partial \xi} \right) A k^3 d\xi \quad 6.6$$

and the mobility

$$\mu = -\frac{e\tau}{m^*} \quad 6.7$$

Note that ξ is the reduced Fermi level equal to E_F/kT . The reduced energy notation is very useful for computation purposes when numerical integrations are performed.

Under the same conditions as for $\alpha(B)$, equation 4.9 for the transverse N.-E. effect simplifies to the following equation:

$$Q_1(B) = \frac{1}{B} \frac{\sigma_{12}^{\theta 11} - \sigma_{11}^{\theta 12}}{\sigma_{11}^2 + \sigma_{12}^2} \quad 6.8$$

In the case of a weak magnetic field, that is when

$B \rightarrow 0$,

$$Q_1 = \frac{\hbar}{e} \frac{\langle \mu \rangle \langle \xi \mu^2 \rangle - \langle \xi \mu \rangle \langle \mu^2 \rangle}{\langle \mu \rangle^2} \quad 6.9$$

From that equation, one will note that in this region of field, the transverse N.-E. coefficient is independent of the field;

it is a constant. It is also independent of the sign of e_i since e_i and μ_i both carry the same sign. This shows again, that the sign of Q_1 depends only on the scattering mechanism.

In the case of a parabolic band, all the bracket terms, $\langle \rangle$, become Fermi integrals.

From equation 6.8, the behaviour of Q_1 , as the magnetic field increases to the strong field region, is not easily seen. Expressions can be found however for the case of a parabolic band and assuming classical statistics. Referring to Tsidil'kovski's book (p. 77, 62T2): When $(\mu B)^2 \ll 1$, the transverse N.-E. field is:

$$E_y = \left(\frac{1}{2} - r\right) a_r \frac{k}{e} \mu B \frac{\partial T}{\partial x} \quad 6.10$$

so that

$$Q_1 = \left(\frac{1}{2} - r\right) a_r \frac{k}{e} \mu \quad 6.11$$

When $(\mu B)^2 \gg 1$,

$$E_y = \left(\frac{1}{2} - r\right) c_r \frac{k}{e} (\mu B)^{-1} \frac{\partial T}{\partial x} \quad 6.12$$

$$Q_1 = \left(\frac{1}{2} - r\right) c_r \frac{k}{e} (\mu B)^2{}^{-1} \quad 6.13$$

The parameter r comes from the definition of the relaxation time used in that reference:

$$\tau = \tau_0 \left(\frac{\epsilon}{kT} \right)^{r - \frac{1}{2}} \quad \text{so that } r = s + \frac{1}{2}$$

In those equations, a_r and c_r are the following:

$$a_r = \frac{3\sqrt{\pi}}{4} \frac{\Gamma\left(\frac{3}{2} + 2r\right)}{\Gamma^2(2+r)} \quad 6.14$$

$$c_r = \frac{16}{9\pi} \Gamma(3-r) \Gamma(2+r) \quad 6.15$$

with the gamma functions:

$$\Gamma(r) = \int_0^{\infty} e^{-x} x^{r-1} dx \quad 6.16$$

The coefficients a_r and c_r have values near unity; they have the values listed in table 6.1 for various values of r , the relation to s is also given in the same table.

It is seen from equation 6.13 that the coefficient Q_1 will decrease to zero as the reciprocal of the square of the magnetic field induction, $1/B^2$.

TABLE 6.1

Values of the parameters a_r and c_r for different values of s .

As of (p. 78, 62T2)

s	r	a_r	c_r
-0.75	-0.25	1.5738	1.3258
-0.50	0	1.1781	1.1318
-0.25	0.25	1.0356	1.0312
0	0.50	1.0000	1.0000
0.25	0.75	1.0278	1.0312
0.50	1.00	1.1045	1.1318
0.75	1.25	1.2273	1.3258
1.00	1.50	1.4000	1.6667
1.25	1.75	1.6308	2.2686
1.50	2.00	1.9328	3.3953

Note

If the reader refers to the literature of the transverse N.-E. effect, he should not be surprised that in the general case of a magnetic field of arbitrary magnitude, many authors use the non-dimensional field ξ_y ,

$$\xi_y = E_y / \left[\frac{k}{e} (dT/\partial x) \right] \quad 6.17$$

rather than the coefficient Q_1 , as a characteristic of the effect. This is because the coefficient Q_1 does not reflect the dependence of the field E_y on the parameter μB , the latter being related intimately to the behaviour of carriers in magnetic fields.

From equations 6.10 and 6.12, E_y is seen to be proportional to μB in weak fields and to $(\mu B)^{-1}$ in strong fields. Therefore, at intermediate field strength, when $\mu B \approx 1$, the function $E_y(\mu B)$ should have a maximum. The value of the mobility μ can thus be found.

6.3. ANALYSIS, RESULTS AND DISCUSSION

The thermoelectric power and its variation with the magnetic field was measured on a number of samples over the alloy range. Figure 6.1 shows the results obtained for 5 of these samples.

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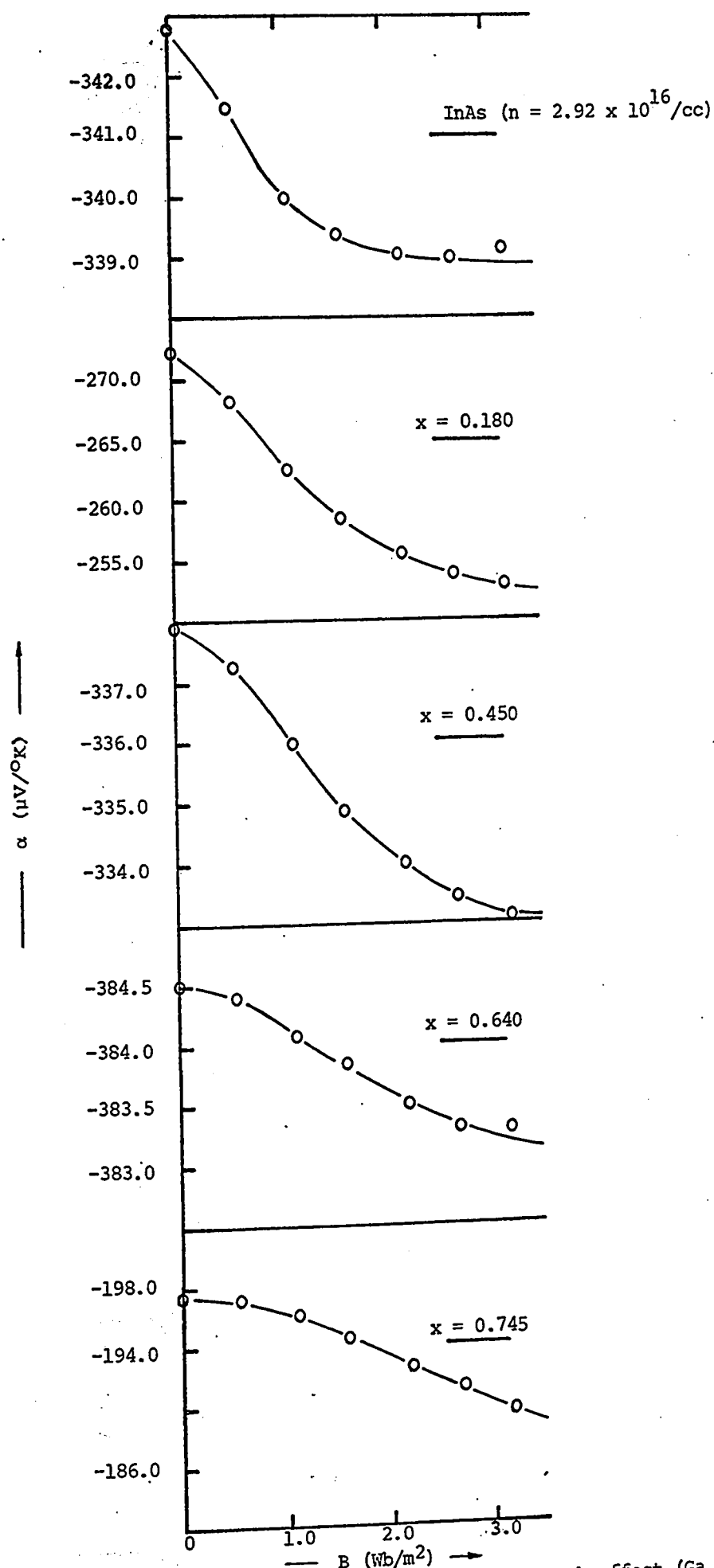


Figure 6.1 Experimental results for the magneto-Seebeck effect ($\text{GaIn}_{1-x}\text{As}$)

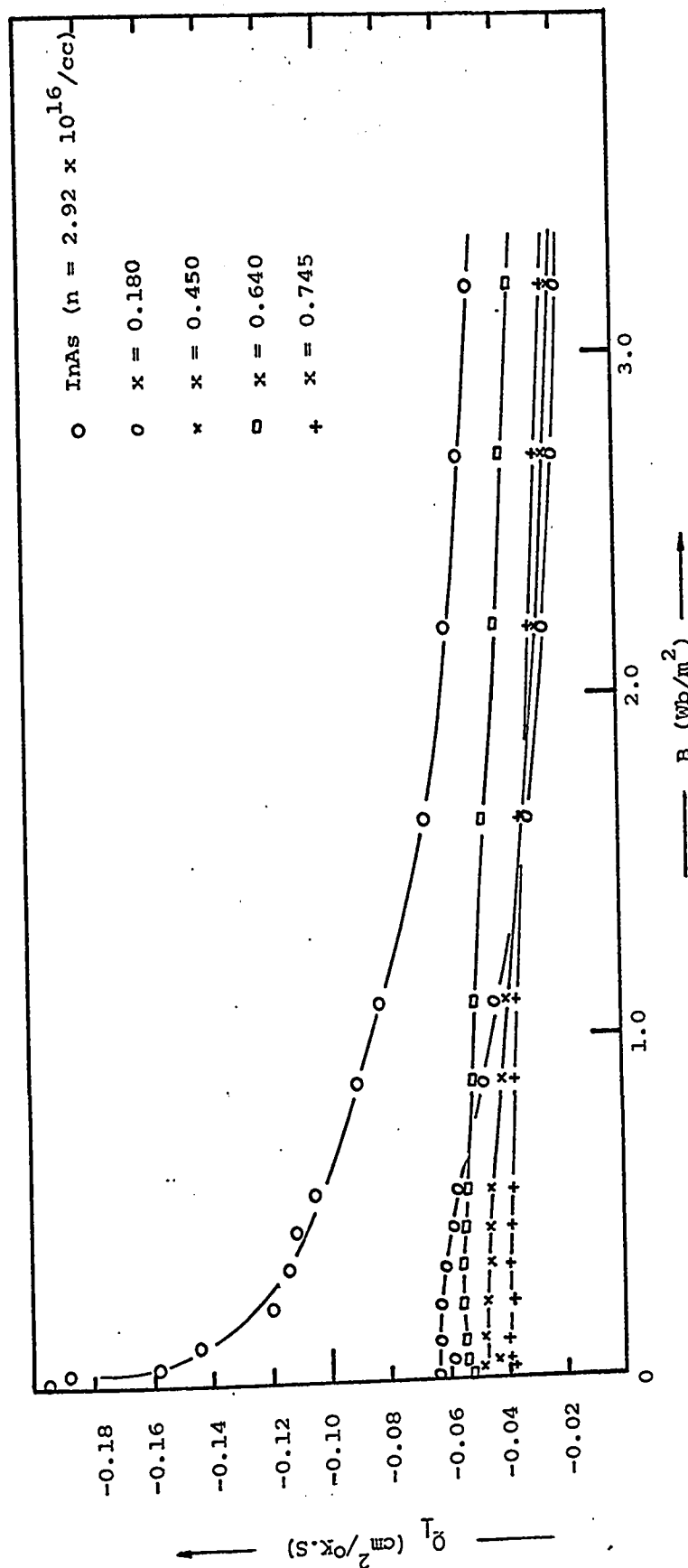


Figure 6.2 Experimental results for the transverse N.-E. effect ($\text{Ga}_x\text{In}_{1-x}\text{As}$)

The transverse N.-E. effect was measured on samples with the following composition: 0.000, 0.180, 0.450, 0.640 and 0.745. Those results are displayed on figure 6.2. The electrical conductivity, which will be needed in the analysis as will be explained later, was also measured on these samples; the values are quoted in table 6.2.

TABLE 6.2

Measured electrical conductivity for 5 samples of the alloy system of $\text{Ga}_{1-x}\text{In}_x\text{As}$.

x	$\sigma (x \cdot 10^4 \Omega^{-1} \text{m}^{-1})$
0.000	1.02
0.180	1.95
0.450	0.95
0.640	0.42
0.745	3.60

The analysis of those measurements has been divided in three sections. The first section shows how the theory described in the previous section was applied in order to calculate the position of the Fermi level, the bottom of the band effective mass and the

scattering parameter.

The second section describes a fitting method developed on curves of $\alpha(B)$ versus B and applied to analyse the transverse N.-E. effect for values of the Fermi level and of the scattering parameter.

The third section gives an account on how the curves of $\alpha(B)$ versus B are fitted assuming specific relaxation times suggested by the values of s . The scattering mechanisms investigated are optical scattering, space-charge and alloy scattering.

6.3.1. CALCULATIONS OF ζ , m^*/m AND s .

6.3.1.1. Assumptions and Procedure

Using the definition of the bracket symbol, equation 6.6, equation 6.4 becomes:

$$\alpha(\infty) = - \frac{\hbar}{e} \left[\frac{\int_0^\infty \left(-\frac{\partial f_0}{\partial \xi}\right) \xi^3 d\xi}{\int_0^\infty \left(-\frac{\partial f_0}{\partial \xi}\right) k^3 d\xi} - \zeta \right] \quad 6.18$$

If $\alpha(\infty)$ is known, the Fermi level can be calculated from that equation provided a model is assumed for k .

If equation 4.13 is replaced in equation 6.18, the bottom

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of the band effective mass will cancel out.

In order to use equation 6.18, the value of $\alpha(\infty)$ has to be found. Figure 6.3 shows the variation of $\Delta\alpha(B)$ with B for three samples of the alloy system. In cases where the saturation value of $\Delta\alpha(B)$ cannot be found from the plots, the limiting value $\Delta\alpha(\infty)$ was found with the aid of an extrapolation method based on an empirical formula first suggested by Shalyt (63S1) for InAs:

$$\Delta\alpha(B) = A_1 B^2 / (1 + A_2 B^2) \quad 6.19$$

where A_1 and A_2 are constants.

This empirical formula has been indirectly suggested by a paper of Rodot (60R2) in which he gives a theoretical justification for a formula of this type in the case of a degenerate electron gas.

In equation 6.19, if B is large, it becomes:

$$\Delta\alpha(\infty) = \frac{A_1}{A_2}$$

Rearranging equation 6.19,

$$\frac{B^2}{\Delta\alpha(B)} = \frac{1}{A_1} + \frac{A_2}{A_1} B^2 \quad 6.20$$

$$= \frac{1}{A_1} + \frac{1}{\Delta\alpha(\infty)} B^2 \quad 6.21$$

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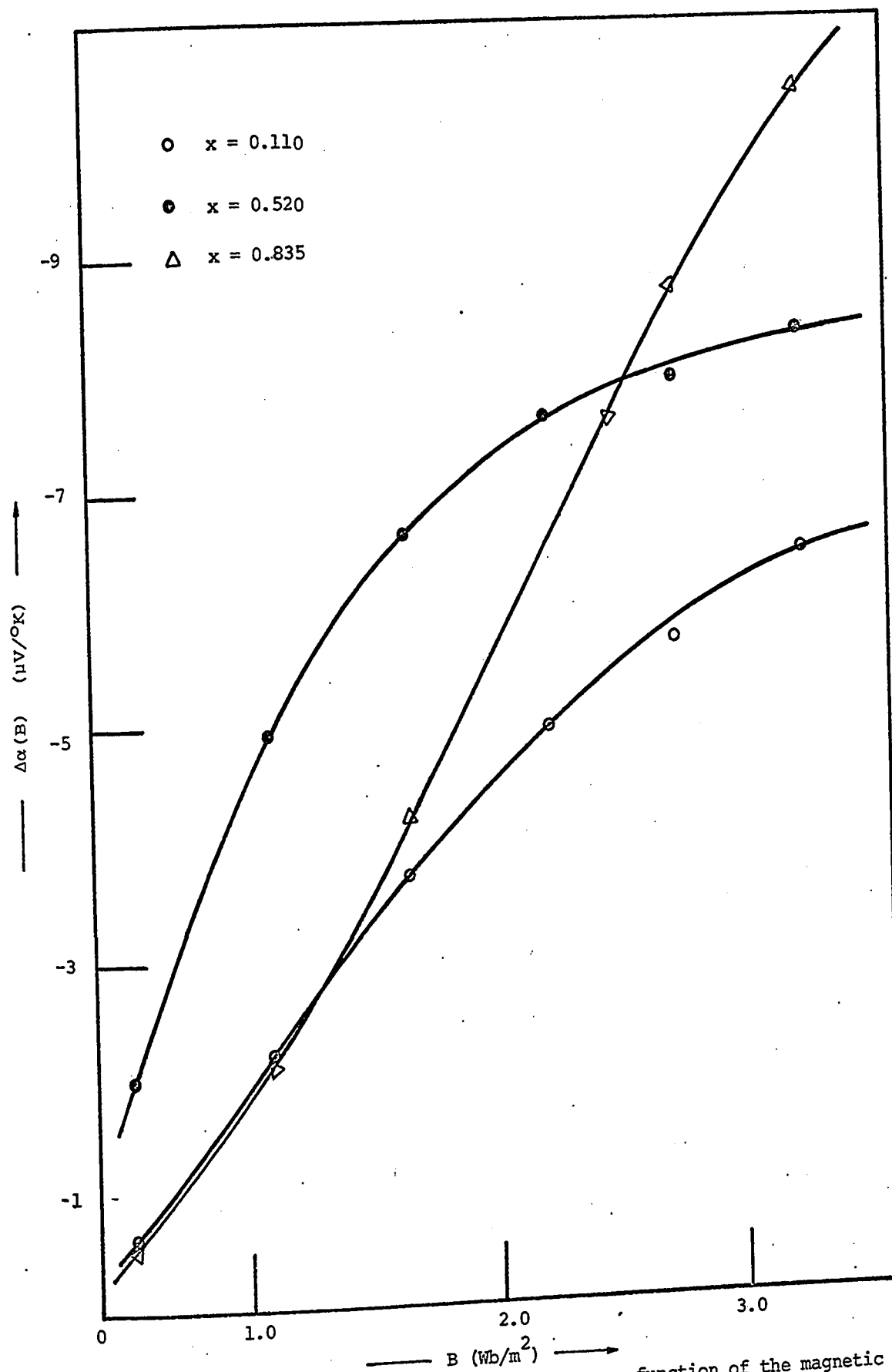
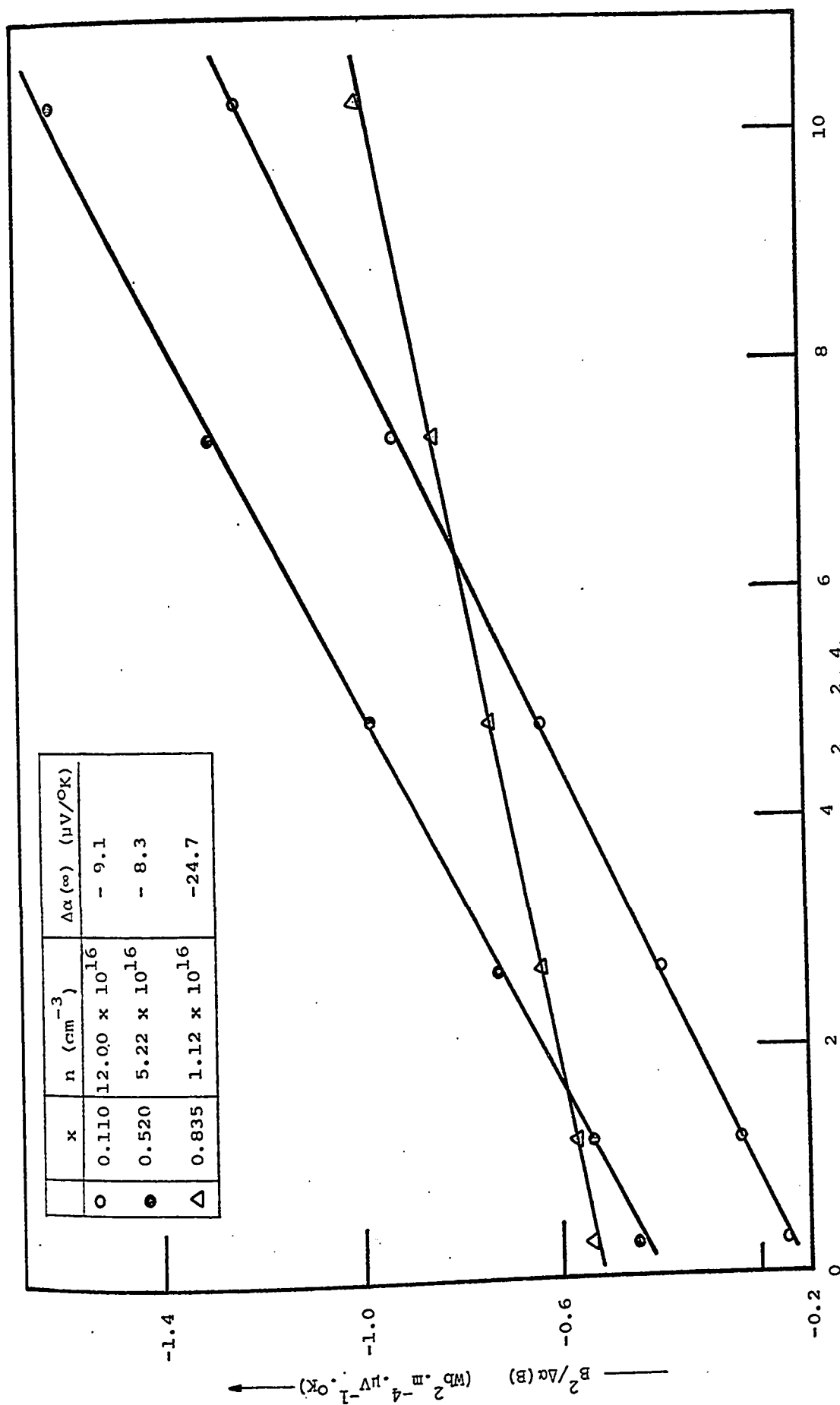


Figure 6.3 Variation of the thermoelectric power as a function of the magnetic field (Longitudinal N.-E. effect)

Figure 6.4 Graph of $B^2/\Delta\alpha(B)$ as a function of B^2

Thus, a plot of $B^2/\Delta\alpha(B)$ as a function of B^2 should provide with a straight line of slope $1/\Delta\alpha(\infty)$. Figure 6.4 shows that indeed one obtains straight lines.

Values for the Fermi level can then be calculated if E_0^* in the Kane model is known. The values used here have been taken from Hall coefficient and electrical conductivity measurements published by Coderre and Woolley (70Cl).

Again, using equation 6.6, equation 6.3 becomes:

$$\alpha(o) = - \frac{k}{e} \left[\frac{\int_0^\infty \left(-\frac{\partial f_o}{\partial \xi}\right) \xi \mu k^3 d\xi}{\int_0^\infty \left(-\frac{\partial f_o}{\partial \xi}\right) \mu k^3 d\xi} - \zeta \right] \quad 6.22$$

Substituting the mobility, equation 6.7, and introducing the "generalized form" of the relaxation time, equation 4.50, one obtains:

$$\alpha(o) = - \frac{k}{e} \left[\frac{\int_0^\infty \left(-\frac{\partial f_o}{\partial \xi}\right) \xi k^{2s-1} \left(\frac{d\xi}{dk}\right)^2 d\xi}{\int_0^\infty \left(-\frac{\partial f_o}{\partial \xi}\right) k^{2s-1} \left(\frac{d\xi}{dk}\right)^2 d\xi} - \zeta \right] \quad 6.23$$

The constant τ_o in equation 4.50 is seen to cancel out, top and bottom.

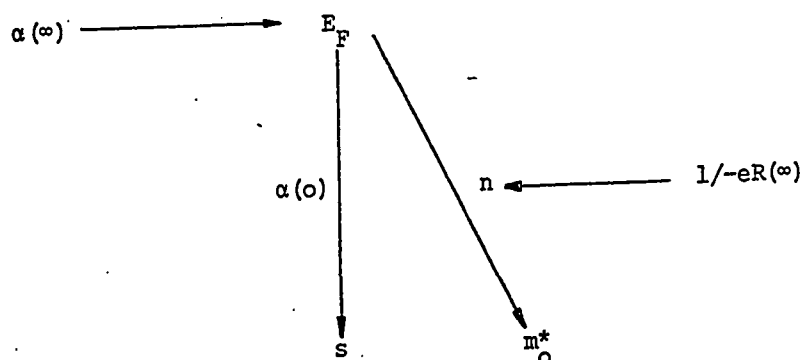
If $\alpha(0)$ is known and the Fermi level, the parameter s can hence be calculated.

Furthermore, including the Kane model in equation 6.5 for the carrier concentration:

$$n = \frac{1}{3\pi^2} \left(\frac{2kT m_o^*}{h^2 E_o^*} \right)^{3/2} \int_0^\infty \frac{e^{\xi-\zeta}}{(1 + e^{\xi-\zeta})^2} (E_o^* \xi + kT \xi^2)^{3/2} d\xi \quad 6.24$$

The carrier concentration being known from the Hall effect measurement and the Fermi level from $\alpha(\infty)$, the bottom of the band effective mass m_o^* can also be calculated.

In résumé, the scheme of the possible calculations is the following:



This method to calculate the parameters involved in equations 6.3, 6.4 and 6.5 has evolved from 1960 to now, in going from equations assuming a parabolic band to those using a non-parabolicity correction.

It has its origin in the fact that Rodot (60R1, 60R2), suggested the form of equation 6.4 for $\alpha(\infty)$. The evolution can be followed in papers by Mochan, Obraztsov and Smirnova (62M2) on InSb, Galavanov, Emel'yanenko and Kesamanly (63G1), Shalyt (63S1) and Korenblit, Mashovets and Shalyt (64K2). In this last reference, the authors investigated the dispersion law of InAs from measurements of $\alpha(\infty)$ and $R(\infty)$; they also studied the scattering mechanism in InAs by plotting a graph of $\alpha(0)$ versus carrier concentration.

This scheme of the calculations has also been used by Dr. M. Aubin in his Ph.D. thesis (69A2).

6.3.1.2. Results and discussion

The results of the calculations of $\alpha(\infty)$ using the empirical relation of Shalyt are given in table 6.3 with the measured values of $\alpha(0)$ and $R(\infty)$. The values of the longitudinal N.-E. effect $\Delta\alpha(\infty)$ are also listed.

The latter is seen to have a negative sign which already tells us that s will be positive if the non-parabolicity does not affect its sign.

The values of $\Delta\alpha(\infty)$ represent only a few percent of $\alpha(0)$; this means that as a first approximation, the Fermi level could be calculated using the value of $\alpha(0)$ instead of $\alpha(\infty)$.

A calculation was made for the case of $x = 0.61$ to find out the sensitivity of ζ and s with respect to the value of $\Delta\alpha(\infty)$. Table 6.4 shows that if $\alpha(\infty)$ is set equal to $\alpha(0)$, this produces a change of 5.6% in the Fermi level, 7.1% in the bottom of the band effective mass and 31.3% in the value of s .

This shows that the parameter s is more sensitive to $\Delta\alpha(B)$ than is the Fermi level, the latter depending mostly on the thermoelectric power itself.

This simple calculation means also that even an experimental error as high as 20% in $\Delta\alpha(\infty)$ would produce changes in ζ and s of about 1 and 6% respectively.

Table 6.5 gives the results of the calculations of the carrier concentration n , the Fermi level E_F , the effective mass at $k = 0$ and of the scattering parameter s , for all the alloys measured. All these calculations were done by numerical integration; these computations as well as those in the following work were performed on an IBM 360 computer, Model 50.

The numerical integrations used Simpson's rule with enough intervals to provide a good accuracy. The summation was done up to a value of energy such that a negligible number of electrons would have an energy greater than this.

The variation of the bottom of the band effective mass with the composition of the alloy is displayed on figure 6.5. The value for InAs agrees with other measurements as published by Aubin and Woolley (68A1).

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TABLE 6.3

Data from the $\text{Ga}_{1-x}\text{In}_x\text{As}$ alloys.

x	$\alpha(0)$ ($\mu\text{V}/\text{deg}$)	$\Delta\alpha(\infty) \equiv$ $ \alpha(\infty) - \alpha(0) $	$\alpha(\infty)$ ($\mu\text{V}/\text{deg}$)	$-R(\infty)$ (cm^3/C)
0.000	-342.8	- 4.2	-338.6	214.08
0.000	-355.7	+ 1.6	-357.3	269.80
0.110	-256.0	- 9.1	-246.9	52.00
0.190	-282.0	- 8.6	-273.4	63.36
0.285	-304.5	- 8.3	-296.2	73.60
0.375	-321.2	- 6.3	-314.9	84.19
0.450	-337.9	- 4.7	-333.2	93.36
0.520	-376.0	- 8.3	-367.7	119.61
0.610	-408.3	- 8.9	-399.4	159.58
0.640	-384.5	- 1.8	-382.7	138.37
0.745	-197.4	-19.0	-178.4	8.89
0.835	-351.6	-24.7	-326.9	55.90

TABLE 6.4

Shows the sensitivity of ζ and s with respect to the value of $\Delta\alpha(\infty)$.

(Data for $x = 0.61$)

IF			VARIATION %
$\alpha(o)$	-408.3 $\mu\text{V}/^\circ\text{K}$	-408.3 $\mu\text{V}/^\circ\text{K}$	
$\alpha(\infty)$	-399.4 $\mu\text{V}/^\circ\text{K}$	-408.3 $\mu\text{V}/^\circ\text{K}$	
$\Delta\alpha(\infty)$	- 8.9 $\mu\text{V}/^\circ\text{K}$	0.0	100.0
THEN			
ζ	- 1.98	- 2.09	5.6
m^*/m	0.0493	0.0528	7.1
s	0.32	0.22	31.3

TABLE 6.5

Computed results from the $\text{Ga}_{1-x}\text{In}_x\text{As}$ alloys .

x	n ($\times 10^{16}/\text{cm}^3$)	ζ (E_F in kT)	m^*_o/m	s
0.000	2.92	- 1.09	0.0213	0.48
0.000	2.31	- 1.33	0.0212	0.41
0.110	12.00	+ 0.21	0.0267	0.52
0.190	9.55	- 0.23	0.0301	0.47
0.285	8.46	- 0.58	0.0339	0.42
0.375	7.43	- 0.86	0.0369	0.36
0.450	6.69	- 1.12	0.0405	0.32
0.520	5.22	- 1.57	0.0459	0.34
0.610	3.91	- 1.98	0.0493	0.32
0.640	4.51	- 1.78	0.0478	0.23
0.745	70.19	+ 1.36	0.0552	0.50
0.835	1.12	+ 1.08	0.0576	0.47

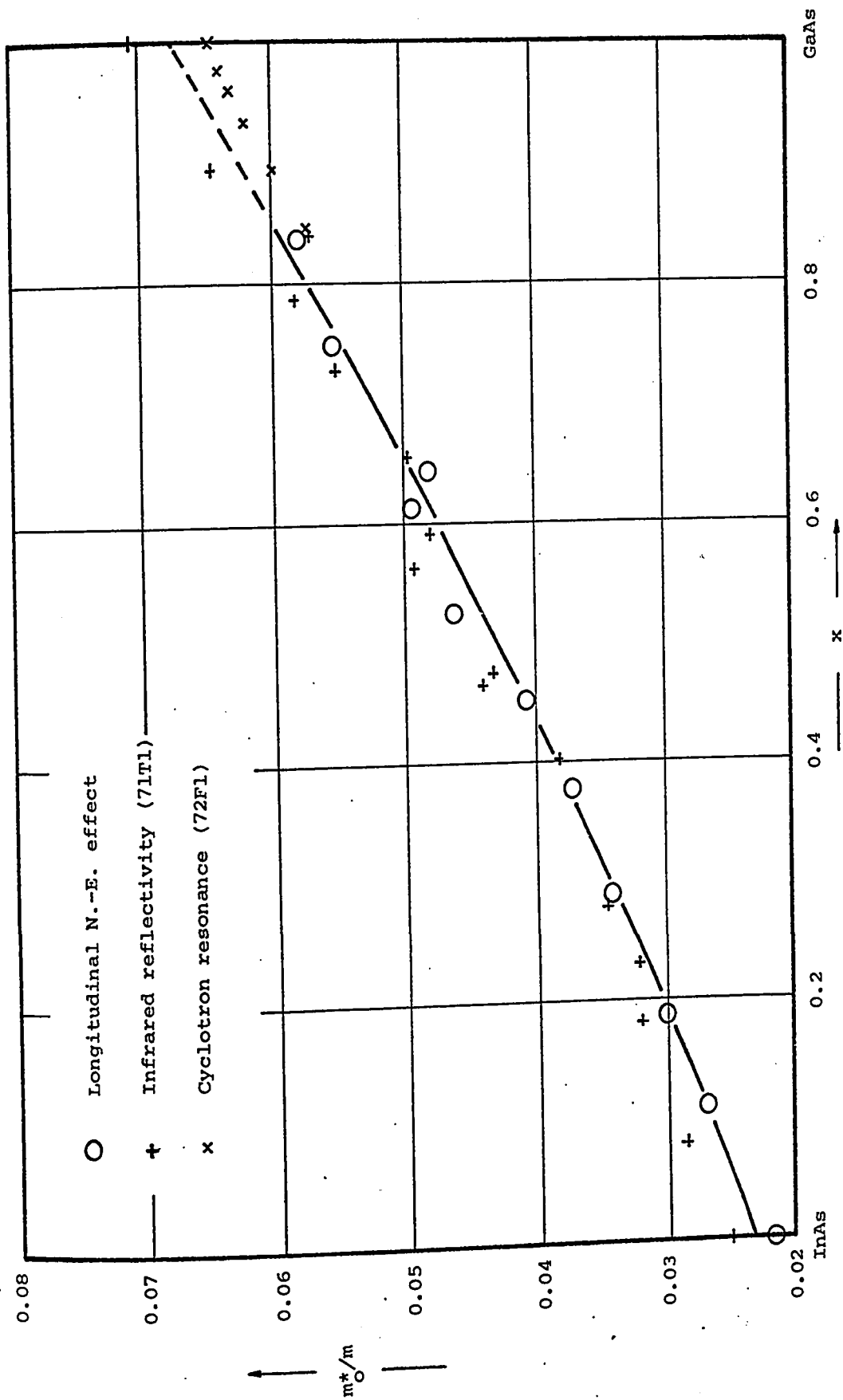


Figure 6.5 Bottom of the band effective mass in $\text{Ga}_x\text{In}_{1-x}\text{As}$ alloys.

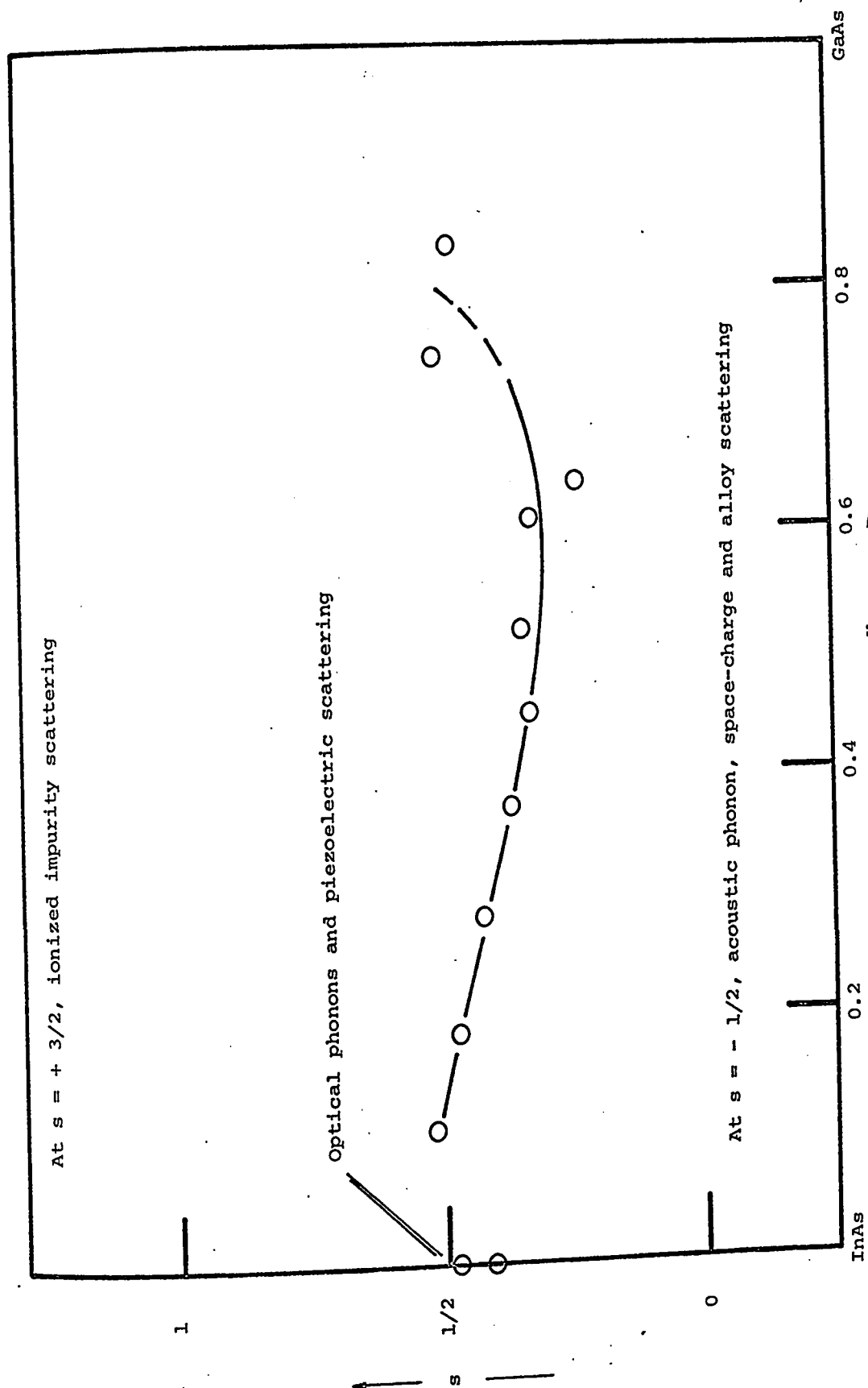


Figure 6.6 Scattering parameter vs composition in $\text{Ga}_x\text{In}_{1-x}\text{As}$

The results are compared with those from infrared reflectivity data of Thomas and Woolley (71T1).

After the present data had been obtained, recent results, from measurements via cyclotron resonance in thin epitaxial films, were reported by Fetterman et al (72F1). The values of effective masses included in figure 6.5, at the high values of x , are those results corrected to room temperature.

Figure 6.6 gives the interesting variation of the scattering parameter s with composition; s is seen to be near $+0.5$ at the InAs end in agreement with other authors (68A1). It then decreases to reach a value of $s \approx +0.3$ around $x = 0.60$.

The values of s agree with the negative sign of the longitudinal N.-E. coefficient; the scattering can therefore be attributed to either optical phonon scattering or piezoelectric scattering on the acoustical branch. Piezoelectric scattering is allowed in this system because both InAs and GaAs have an asymmetric charge distribution and no center of symmetry. This scattering has been pointed out (63S1 and 64K2) as being present in InAs at $T = 77^{\circ}\text{K}$ for samples of low carrier concentrations. In some recent work by Rode (70R1), a numerical iterative method is used to solve the Boltzmann equation; it is applied to pure III-V semiconductors (GaAs, GaSb, InP, InAs, InSb). These compounds were investigated for the possible presence of polar mode, "deformation potential" acoustic and piezoelectric scattering. It is shown that piezoelectric scattering becomes just noticeable ($\sim 10\%$) at 150°K except for GaAs for which it is the dominant mobility-limiting mechanism below 60°K . In some later work, Rode (71R1), included an

arbitrary electron degeneracy as well as scattering by ionized impurities and heavy holes. A similar conclusion was reached. At room temperature, piezoelectric scattering is therefore ineffective, leaving only the mode of optical scattering.

6.3.2. THEORETICAL FIT TO THE CURVES OF α VS B AND INTERPRETATION OF THE TRANSVERSE N.-E. EFFECT

6.3.2.1. Validity and procedure

The method of analysis described in section 6.3.1. relies on two values of $\alpha(B)$. One is experimental, $\alpha(0)$, and the other, $\alpha(\infty)$, is determined with the use of an empirical law.

It was decided, therefore, to use the whole variation of the effect with the magnetic field and to obtain a theoretical fit to that curve by varying the values of the Fermi level and of the scattering index.

This test of the method described in section 6.3.1. has never been made although it has been extensively used by many authors as mentioned previously. Also, the transverse N.-E. effect can be more easily analyzed if a method is developed so as to fit the whole experimental curve. This effect is subjected to a larger experimental error, than the magneto-Seebeck is, because the measurements of the transverse N.-E. voltage require the registration of very small voltages. Hence

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extrapolations to values of $Q_1(0)$ are therefore less precise.

Looking back at equation 6.1 for $\alpha(B)$, it can be seen that equations 6.2, 6.6 and 6.7 have to be used in order to obtain a theoretical curve. The relaxation time τ which is needed in equation 6.7 is again defined by equation 4.50 except that in this case, the constant τ_0 does not cancel out. Appendix 6.1 shows how the value of τ_0 can be calculated using the electrical conductivity.

This method of using the complete experimental curve, instead of only 2 points, has the very important advantage that if, for example, a value of $s = +\frac{1}{2}$ is found from $\alpha(0)$, this meaning that optical phonon scattering is probably present, a relaxation time proper to this mechanism can be inserted in the theoretical calculations and a fit can be made to both of α vs B and Q_1 vs B over the whole curves. Also, this method will not use any empirical law for the determination of the Fermi level.

The procedure followed in this approach will now be described. One experimental point is chosen, for example, $\alpha(B_i)$. Curves of α versus $\zeta = E_F/kT$ are plotted for different values of s . See figure 6.7. The values (ζ, s) corresponding to the experimental value $\alpha(B_i)$ are noted. This is repeated for many values of B . A graph of s as a function of ζ is finally obtained for different values of the magnetic field induction B , figure 6.8. The intersection of all the curves, if it exists, is the best possible fit. Note that the area at the intersection also gives an indication as to the quality of the fit.

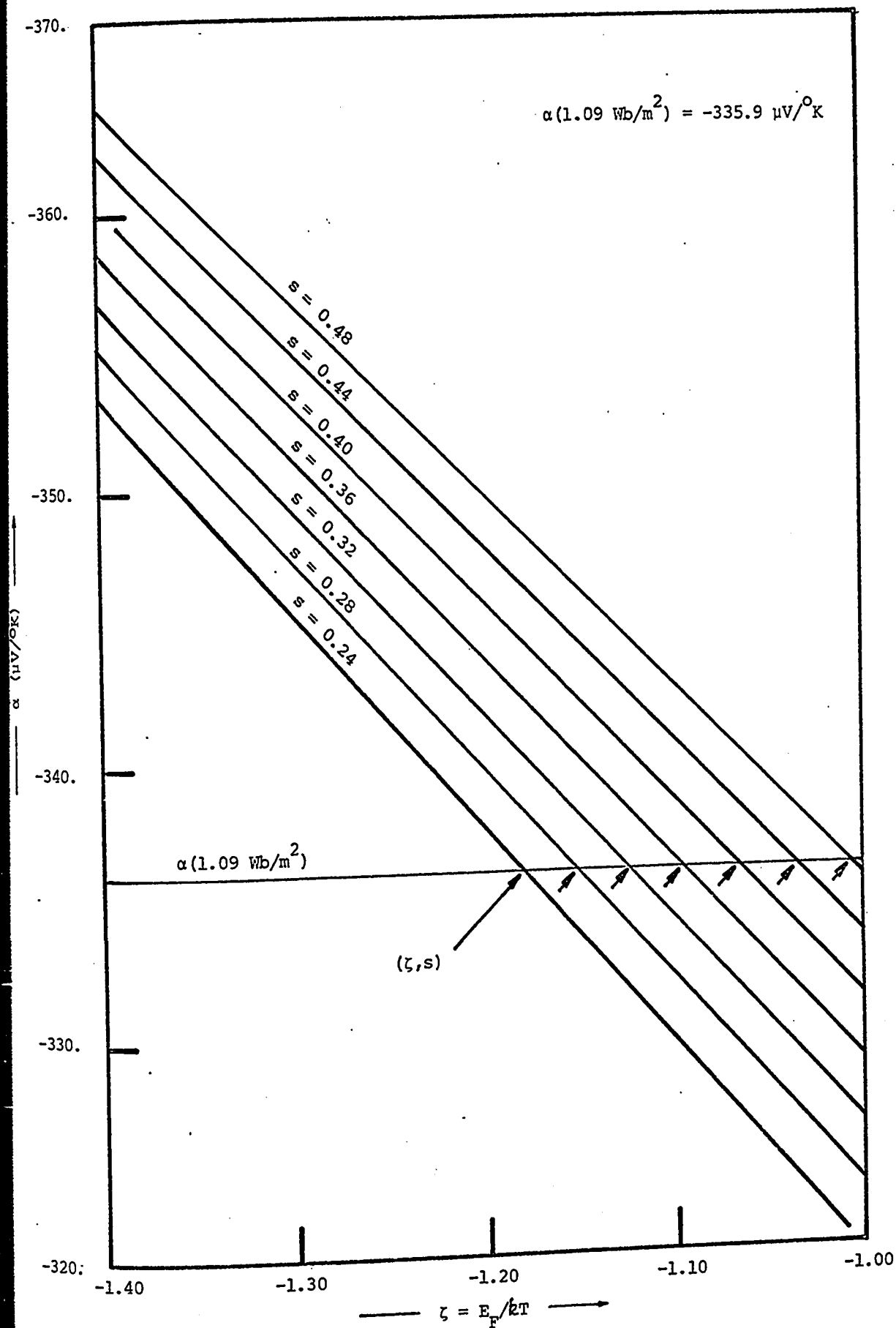


Figure 6.7 Thermoelectric power versus Fermi level for $x = 0.45$ (computed)

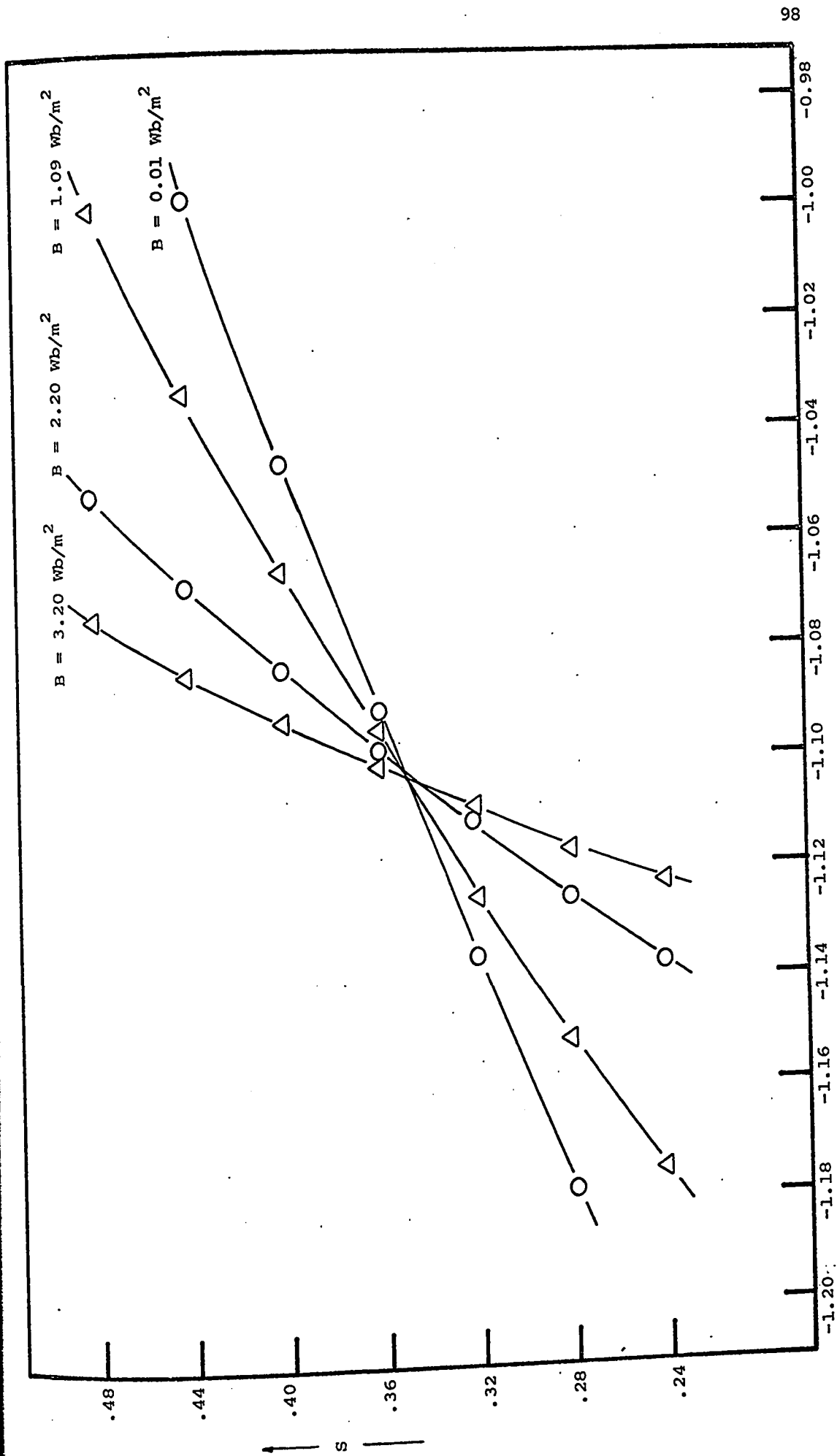


Figure 6.8 Scattering parameter versus Fermi level (for $x = 0.45$)

This is also valid for the curves of Q_1 versus B . This fitting method was devised to save some computer time since the programs already required lengthy calculations.

Only 2 parameters, E_F and s , were used because it seemed illogical to fit with more parameters, the values of m_0^* from the previous analysis having been confirmed by other measurements.

6.3.2.2. Results and discussion

a) Theoretical fit to the curves of α vs B

The results of the best theoretical possible fit to the measurements of the thermoelectric power as a function of the magnetic field are shown in figure 6.9 for five samples of the $\text{Ga}_{1-x}\text{In}_x\text{As}$ alloy system. Figure 6.10 is an enlarged scale, for $x = 0.450$, from which figure 6.9 originates.

Table 6.6 gives the values of the parameters ζ and s , and compares them with those from $\alpha(\infty)$ and $\alpha(0)$ of section 6.3.1. The agreement is good showing that the method described in section 6.3.1., using only two points, $\alpha(0)$ and $\alpha(\infty)$, is indeed a good approximation to the fitting method.

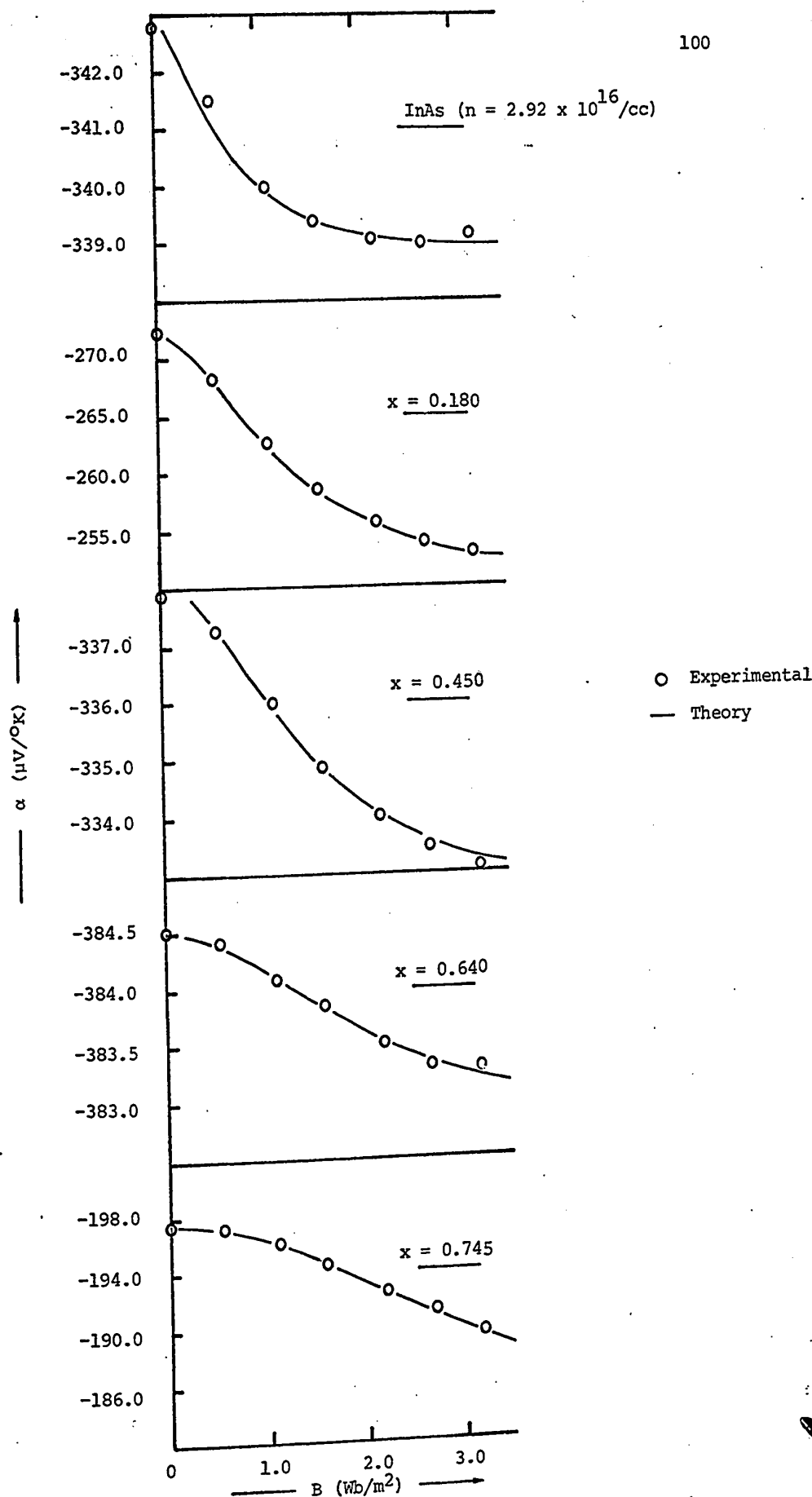


Figure 6.9 Theoretical fit to the magneto-Seebeck effect ($\text{Ga}_x\text{In}_{1-x}\text{As}$)

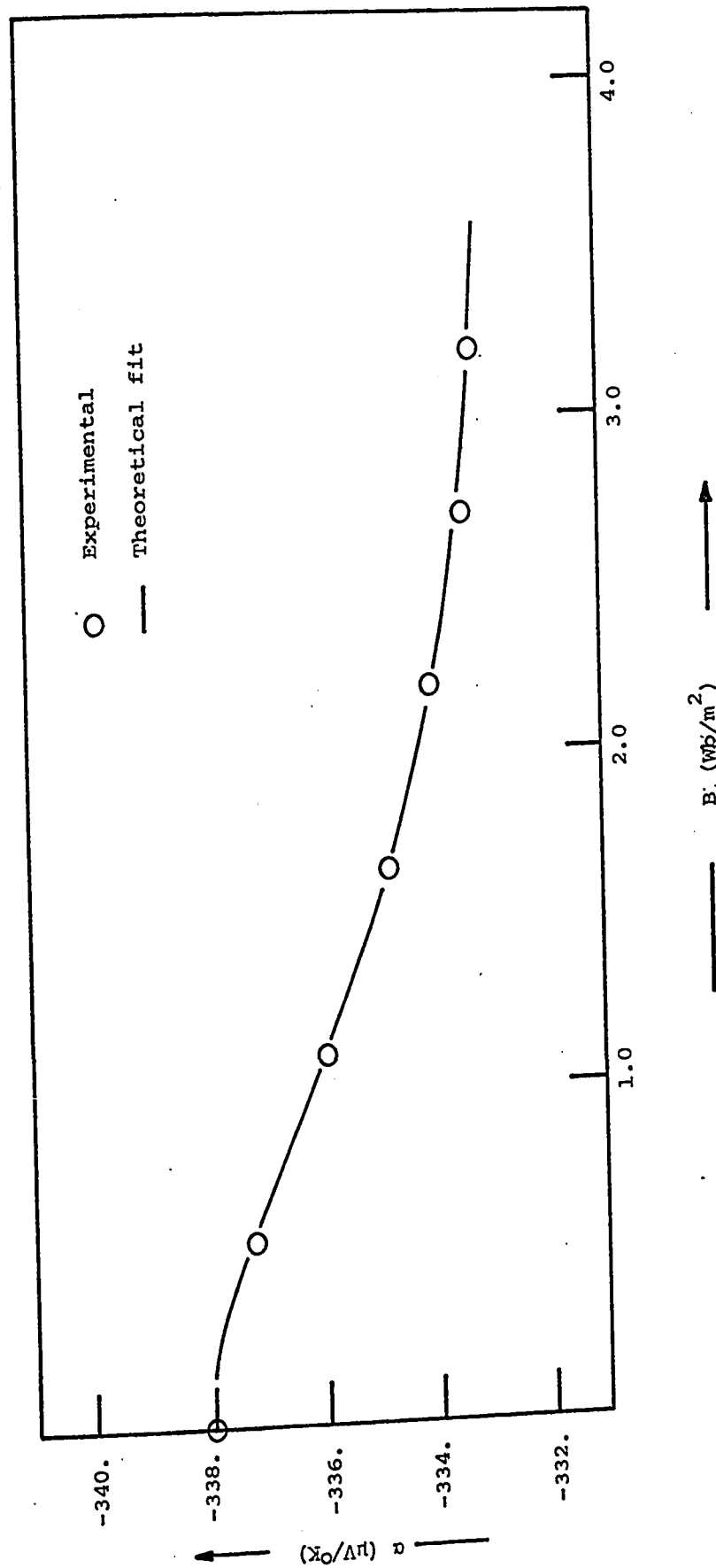


Figure 6.10 Fit to the magneto-Seebeck effect for $x = 0.450$

TABLE 6.6

Comparison of the parameters ζ and s
 calculated either from $\alpha(\infty)$ & $\alpha(0)$ or from
 a fit to the experimental curves of α vs B .

X	ζ		s	
	$\alpha(\infty)$	Fit	$\alpha(0)$	Fit
0.000	-1.085	-1.082	.48	.49
.180	+0.136	+0.154	.64	.66
.450	-1.118	-1.103	.32	.35
.640	-1.780	-1.773	.23	.25
.745	+1.360	+1.323	.50	.49

b) Interpretation of the transverse N.-E. effect

Assuming at the start that the inhomogeneities did not contribute to the transverse N.-E. coefficient, a theoretical fit was made to the curve of Q_1 vs B for $x = 0.450$. The results are shown on figure 6.11. With the values of ζ and s given in table 6.6, the theoretical curve is way off the experimental curve. A fit was possible for $\zeta = -0.300$ and $s = 0.450$. When $x = 0.000$ was analyzed, it was impossible to obtain anything near a fit.

Before analyzing the measurements of this effect, one should know that the material usually contains some inhomogeneities which affect the observed physical phenomenon whether they are micro-inhomogeneities (66D1) or inhomogeneities of mean dimensions larger than the mean-free path of the electrons (68A3). If one tries to fit the experimental data without removing the contribution of the inhomogeneities, in all cases except under weak field conditions, it is impossible to obtain reasonable values of the fitting parameters. It is possible under weak field conditions because depending on the nature of the inhomogeneities, the relative importance of these might increase with increasing magnetic field. Therefore, in weak fields,

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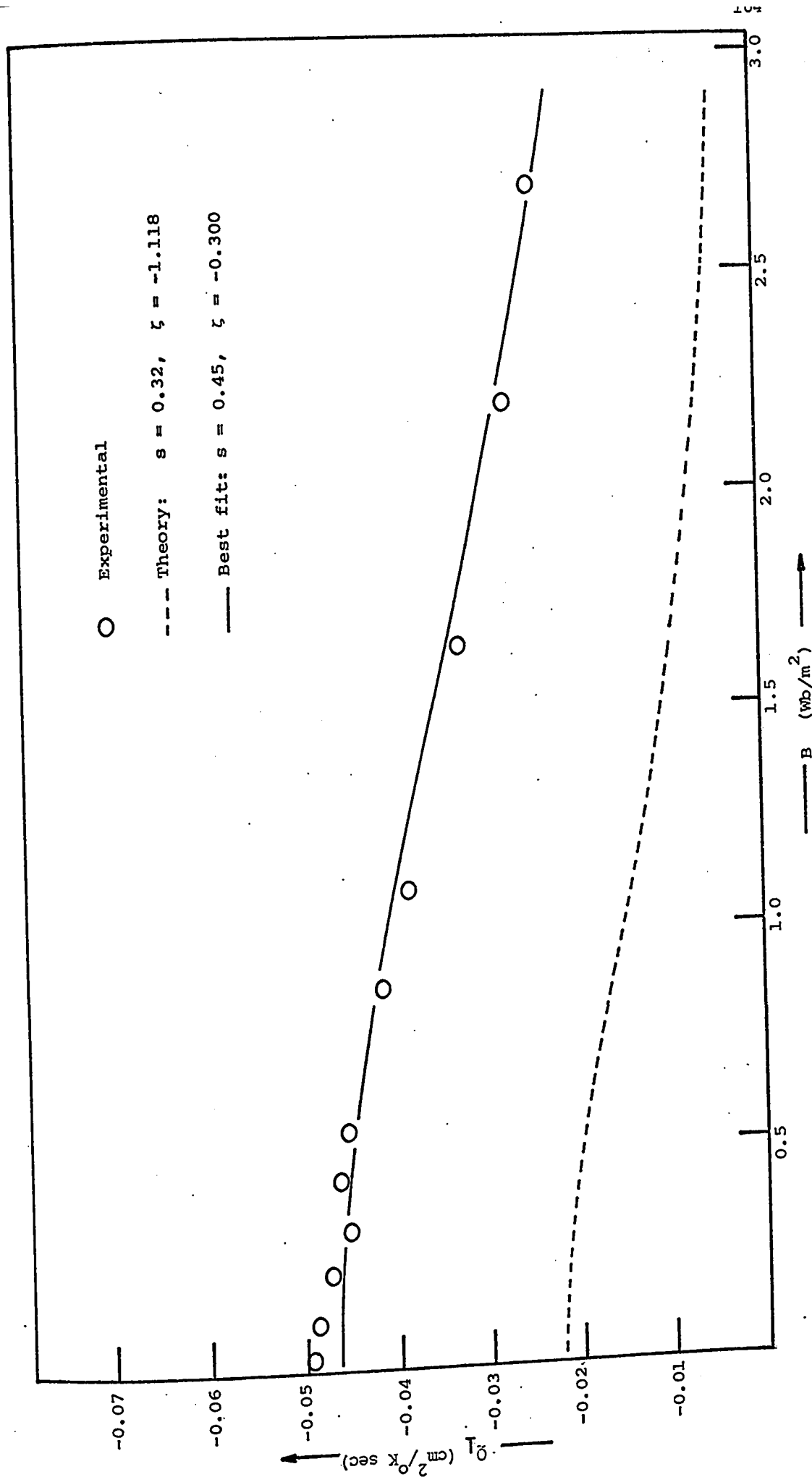


Figure 6.11 Fit to the transverse N.-E. coefficient for $x = 0.450$

one may consider in first approximation that the contribution from the inhomogeneities is negligible. The sample $x = 0.745$ being the one with the lowest mobility, the region of the measurements stands as $\mu B \leq 1$; the fit to be shown later for that sample was made without taking into account the inhomogeneities. The parameters ζ and s will be seen to be reasonable.

The presence of inhomogeneities becomes obvious if one considers the equation for $Q_{\perp}$ in the case of a parabolic band and spherical energy surfaces. In strong magnetic fields, equation 6.13 shows that $Q_{\perp}$ should vary as $1/B^2$ in the classical region.

Figure 6.2 gave the experimentally observed values of $Q_{\perp}$ as a function of the magnetic field; $|Q_{\perp}|$ does not decrease to zero as $1/B^2$ but rather it seems as though it wants to saturate above the zero axis.

This phenomenon was studied by Drichko and Mochan (66D1); they showed that a contribution of the inhomogeneities to the measured transverse N.-E. coefficient is important even in the case of single crystals of InSb which were homogeneous in potential distribution along and across the ingot within 2% at liquid nitrogen temperature. They found that for all their samples, at large fields, all values of $Q_{\perp}$ are of the same sign and differ from one another by not more than 20%. Such behaviour cannot be explained by classical theory. The fact that

this common limit does not vary with temperature indicates that for fairly strong magnetic fields, scattering only has a slight influence on the transverse N.-E. effect.

Herring (60H1) has reviewed the influence of various types of inhomogeneities on the galvano-magnetic effects and on the thermo-emf. Kudinov and Moizhes (66K1) have expanded Herring's theory on the thermomagnetic effects in strong magnetic fields. Agaev, Mosanov and Ismailov (68A3) found that it was possible to separate the physical effect from the effect of inhomogeneities when these are of such a nature so as to give rise to circulating currents. These currents interact with the magnetic field and produce a Hall emf. This emf is superimposed on the transverse N.-E. emf. Consequently, one measures the sum of the transverse N.-E. coefficient and a contribution due to inhomogeneities:

$$Q_{\perp} \text{ (measured)} = Q_{\perp} \text{ (true)} + Q_{\perp} \text{ (inhomogeneities)}$$

Furthermore, they assumed that $Q_{\perp}$ (i) is independent of the magnetic field not only in the strong field region but over the whole range; this is justified since $Q_{\perp}$ (i) depends on B only through the Hall coefficient R and if the dependence of R on B is weak, as a first approximation this turns out to be quite valid.

The true transverse N.-E. coefficient is then the difference between the coefficient measured in weak and in strong field.

This approach will be used here rather than that of Drichko and Mochan (66D1). These authors in their work on InSb measured

the transverse N.-E. coefficient in a magnetic field of induction varying from 0 to 1.5 Wb/m^2 . Since a value of B equal to $\sim 0.2 \text{ Wb/m}^2$ already corresponds to a strong magnetic field, they were able to extrapolate part of the curve ($0.6 - 1.5 \text{ Wb/m}^2$) relating the values of $Q_{\perp}$ with B to the range of values of B below 0.6 Wb/m^2 . The difference between the measured and extrapolated curves was chosen as the true dependence. Such an analysis is impossible in this case because the region of measurement covered in the strong field range is not enough to extrapolate to lower but still high fields.

Figure 6.12 gives an example of the approach used to remove the contribution from the inhomogeneities. The value of $Q_{\perp} (i) = \text{constant}$, was found to be the one which satisfied the equation

$$Q_{\perp} (\text{true}) = Q_{\perp} (\text{measured}) - \text{constant}$$

and for which the fit to $Q_{\perp}$ vs B was the best possible one.

Figure 6.13 shows the curves of $Q_{\perp} (\text{true})$ versus the magnetic field induction for the five samples of the alloy system on which this measurement was made. The associated theoretical fit is calculated using equation 6.8 as it was done for the case of α vs B. The values of the fitting parameters ζ and s are given in table 6.7 where they can be compared with the results from the analysis on the magneto-Seebeck effect.

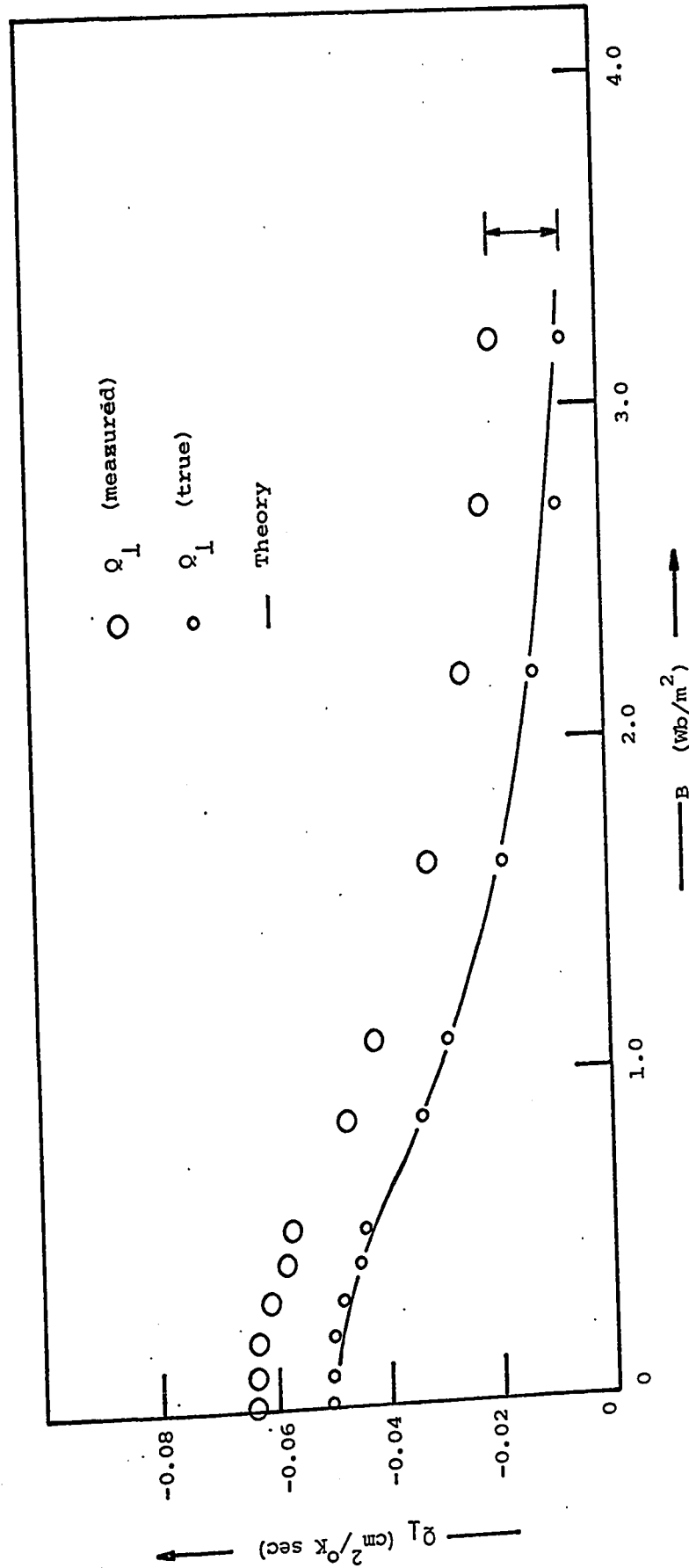


Figure 6.12 Example of the method used to fit the transverse N.-E. coefficient ($x = 0.180$)

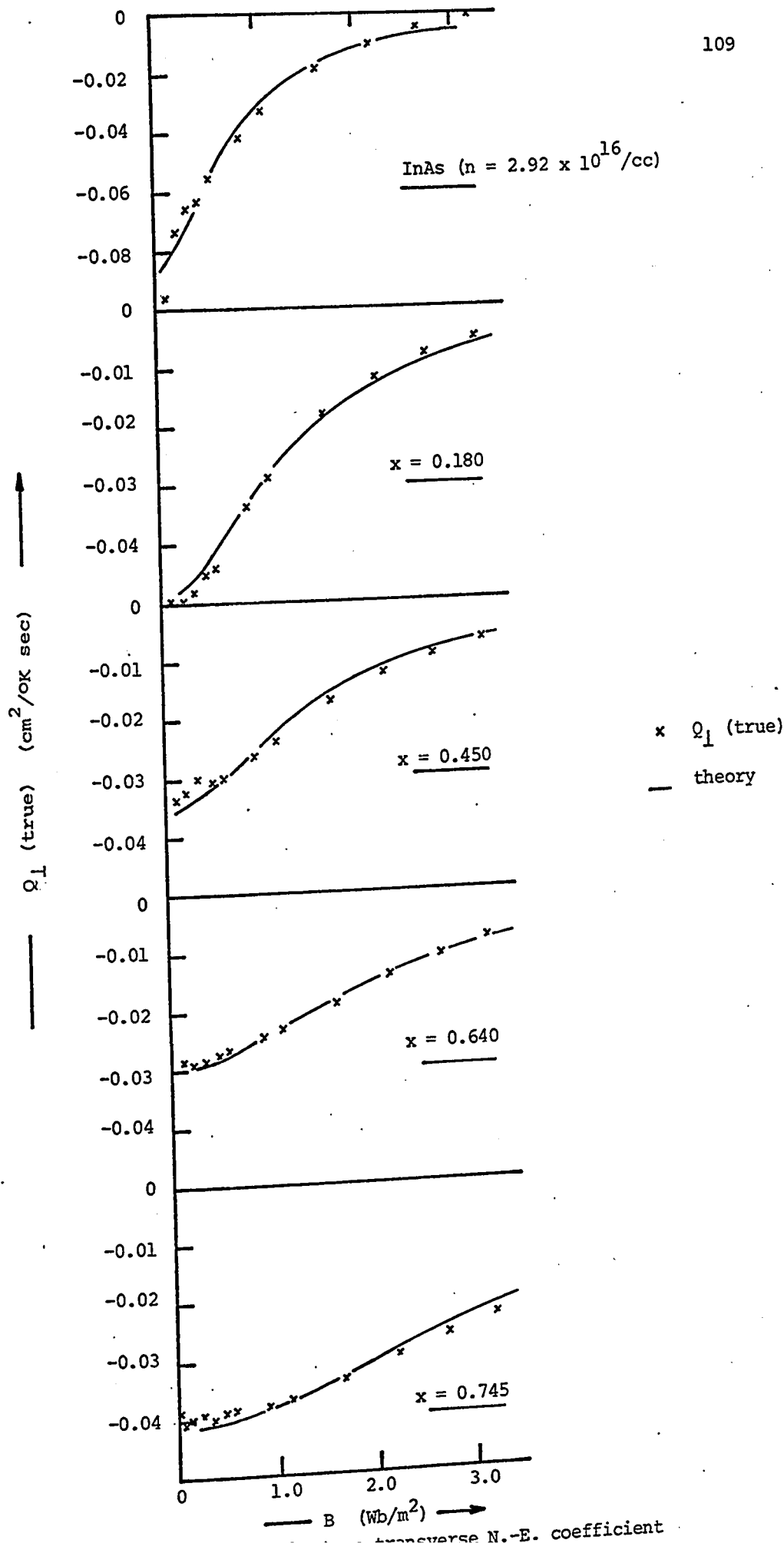


TABLE 6.7

Results on 5 samples of $\text{Ga}_x\text{In}_{1-x}\text{As}$

x	n $\times 10^{16}/\text{cc}$	$\zeta = \frac{E_F}{kT}$ FROM			s FROM		
		$\alpha(\infty)$ ($\mu\text{V}/^\circ\text{K}$)	FIT ON L.N.-E.	FIT ON T.N.-E.	$\alpha(0)$ ($\mu\text{V}/^\circ\text{K}$)	FIT ON L.N.-E.	FIT ON T.N.-E.
0.000	2.92	-1.085	-1.082	-0.820	.48	.49	.52
0.180	10.40	+0.136	+0.154	+0.154	.64	.66	.47
0.450	6.69	-1.118	-1.103	-1.103	.32	.35	.34
0.640	4.51	-1.780	-1.773	-1.773	.23	.25	.30
0.745	70.19	+1.360	+1.323	+1.323	.50	.49	.45

A good agreement is found and the values of the scattering parameter still indicate the same scattering mechanism: optical phonon. The negative sign of Q_1 (true) is in agreement with this conclusion.

It is of interest to mention that in both cases for $\Delta\alpha$ and Q_1 , if they are calculated using a parabolic band, the sign remains negative; this overrules the possibility of the negative sign being due to the non-parabolicity of the investigated material. This was calculated for InAs, $n = 2.92 \times 10^{16}/\text{cc}$, since it is slightly more non-parabolic than GaAs. It can be seen from figure 6.14 that both coefficients are negative for a parabolic band; if a more pronounced non-parabolicity would exist, the sign would turn positive.

The use of equation 4.50 describing the relaxation time has been extensively criticized by Zawadzki and Szymanska (71Z1). This is because, when τ is defined as:

$$\frac{1}{\tau} \propto \rho(E) W(E) \quad 6.25$$

where

$\rho(E)$ is the density of states and

$W(E)$ the scattering probability,

the non-parabolicity should be taken into account in both of $\rho(E)$ and $W(E)$, not only in $\rho(E)$ as is the case for formula 4.50.

However, this is important at high electron concentrations and it is shown in (71Z1) that especially when scattering by ionized impurities is present, this leads to some error in the thermomagnetic effects. Since low carrier concentrations are dealt with here and

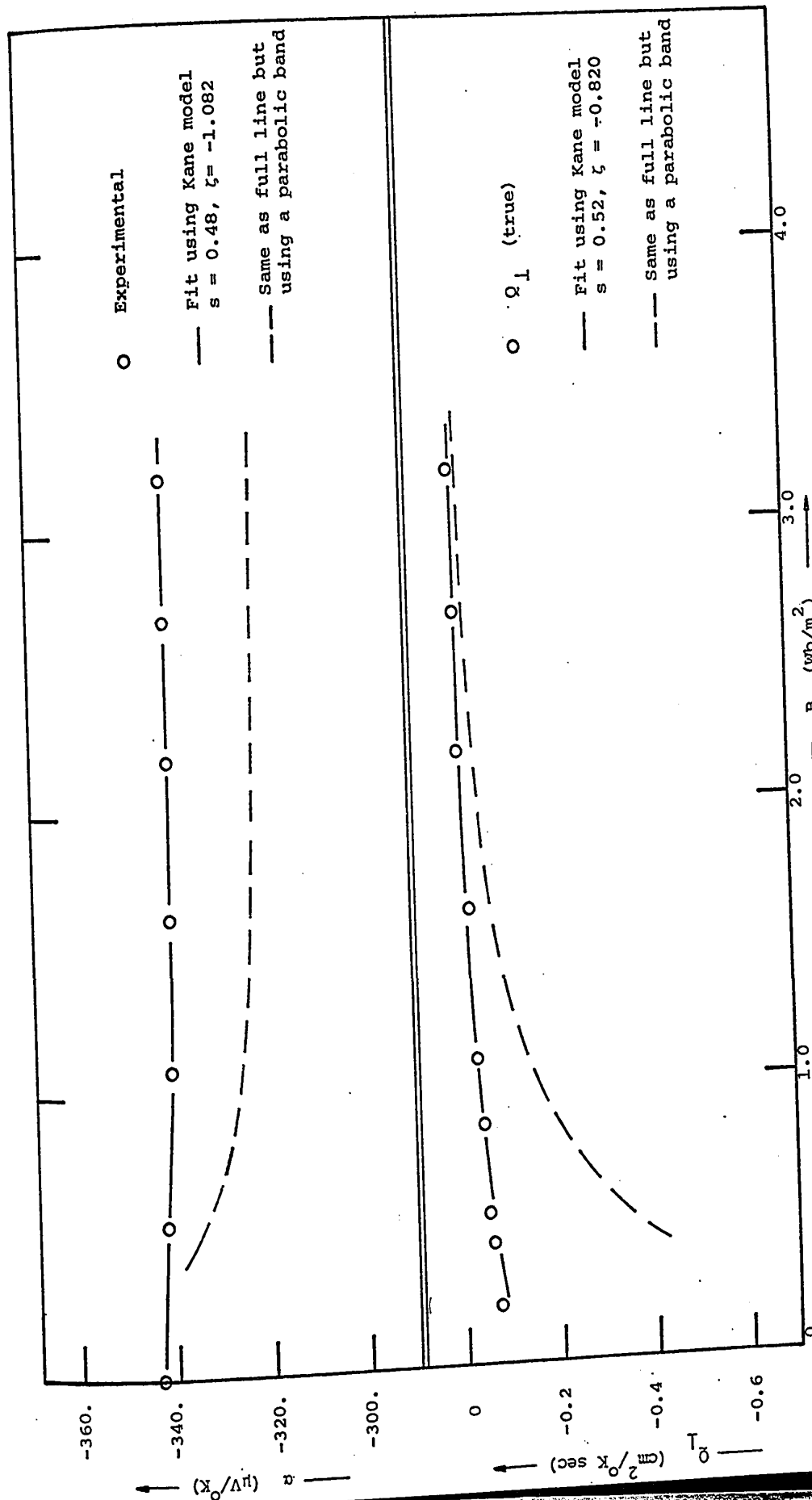


Figure 6.14 Effect of non-parabolicity on the signs of $\Delta\alpha$ and Q_L (InAs, $n = 2.92 \times 10^{16}/\text{cc}$)

ionized impurities have a negligible effect, the use of equation 4.50 is perfectly valid.

The next section, section 6.3.3., will study more closely the possible scattering mechanisms in the alloy system using the relaxation times of specific scattering mechanisms instead of the "generalized form" equation. A distinction needs to be made at this point.

In relation to the inhomogeneities discussed previously, Agaev et al (68A3) mention that the separation of the effect of the inhomogeneities from the physical effect was possible for some types of inhomogeneities only. The following examples are given: layered distribution of impurities in a crystal, crystals with regions having different impurity concentrations, surface layers, electrical (thermal) contacts with a sample, etc. The reader should refer to S. Rosenbaum's thesis (72R1) for further information on the possible nature of inhomogeneities.

From this point on, inhomogeneities of the type just mentioned will be distinguished from alloy or space-charge scattering. Alloy and space-charge scattering will not be called inhomogeneities even though they do represent minor inhomogeneities.

6.3.3. STUDY OF THE POSSIBLE SCATTERING MECHANISMS

Now that the results of both measurements of the longitudinal and transverse N.-E. effects have been interpreted, it is the purpose of this section, to extend the study of figure 6.6. This figure showed

a decrease in s with increasing composition. The behaviour of s means that a scattering mechanism characterized by a negative value of s is having an increasing influence as x increases; it, therefore, imposes a further limitation on the mobility of the carriers.

The possible scattering mechanisms characterized by a negative s are acoustic scattering (deformation potential), alloy scattering and space-charge scattering. They all have a value of s equal to $-\frac{1}{2}$.

Theoretical calculations of Varshni (71V1) and the work of Rode (70R1, 71R1), mentioned earlier, show that acoustic scattering is negligible in III-V compounds. In the work of Rode (70R1), the deformation potentials used are 7.0 and 4.9 eV for GaAs and InAs respectively; in his later paper (71R1), a value of 11.5 eV was used for InAs. Rode also mentions that although the deformation potential values may be in considerable error, the mobility is fairly unaffected because acoustic scattering is quite weak.

Alloy scattering would be the plausible scattering mechanism to hold responsible for a reduction of mobility; this agrees with the predictions of Tietjen and Weisberg (65T1). Their predictions were also correct for the systems of alloys $\text{InAs}_{1-x}\text{Sb}_x$ and $\text{GaIn}_{1-x}\text{Sb}_x$ as can be seen from the results of Aubin and Woolley (68A1, 69A1); the calculated values of s show no continuous or monotonic decrease of s with x . One knows however, that since the mobility due to space-charge scattering has a $T^{-1/2}$ temperature dependence (62W1) which resembles

the mobility due to alloy scattering, it is impossible to distinguish between the two unless an alloy is truly homogeneous. The measurements of the transverse N.-E. effect have shown that the alloys contain some types of inhomogeneities, the nature of which is hard to pinpoint. Nevertheless, both scattering mechanisms will be investigated and a discussion of the results will follow.

6.3.3.1. Procedure

A theoretical fit will be made to the experimental curves of α vs B; the analysis will include specific scattering mechanisms. Because the curves of α vs B are more reliable, it is considered unnecessary to also fit the curves of Q_1 (true) vs B.

Three samples were chosen for this investigation, $x = 0.000$, 0.450 and 0.640. InAs was chosen because alloy scattering is not present and only one scattering mechanism should be needed: optical phonon scattering. If a reasonable fit is found for InAs, a similar approach can be used on the samples in the middle of the alloy range including alloy scattering or space-charge scattering.

When more than one scattering mechanism is present, the resultant relaxation time can be written as:

$$1/\tau = 1/\tau_1 + 1/\tau_2$$

and the resultant mobility:

$$\frac{1}{\mu} = \frac{1}{\mu_1} + \frac{1}{\mu_2} \quad 6.27$$

In order to calculate the percentage contribution of the individual scattering mechanisms to the total scattering, the ratios μ/μ_1 and μ/μ_2 can be calculated.

As for the effective scattering parameter associated with the resultant relaxation time, it is the author's interest to test a relation suggested by Zawadzki and Szymanska (71Z1) of the form:

$$s_{\text{eff}} = (\mu/\mu_1) s_1 + (\mu/\mu_2) s_2 \quad 6.28$$

(valid for degenerate materials only)

If equation 6.28 is fairly valid, one should also be able to estimate the resultant longitudinal N.-E. coefficient in the following way:

$$\Delta\alpha = (\mu/\mu_1) \Delta\alpha_1 + (\mu/\mu_2) \Delta\alpha_2 \quad 6.29$$

A discussion of the choice of the different parameters needed for this analysis follows with the results and discussion. A few comments are also included in relation to equations 6.28 and 6.29.

6.3.3.2. Results and discussion

Figure 6.15 shows the experimental curve of α vs B for InAs; the theoretical curve including only optical scattering, curve 1, is seen to be higher than the experimental one, at low fields. The relaxation time used is described by equations 4.29 to 4.32 for non-parabolic bands. The needed parameters used can be found in table 6.8. The energy of the longitudinal optical phonons was taken from recent far infrared reflectivity measurements made at room temperature by Lucovsky and Chen (70L1) on $\text{Ga}_{1-x}\text{In}_x\text{As}$. The choice of the dielectric constants was the largest difficulty; a number of references having been consulted, the values used by Rode (71R1) for InAs, were finally adopted.

Even if the high frequency dielectric constant κ_∞ , chosen as 12.25 for InAs, which is the parameter showing the most dispersal in value in the consulted references, was varied to 10.2, this did not provide with a better theoretical fit although the relaxation time used is proportional to $(1/\kappa_\infty - 1/\kappa_0)$.

The discrepancy between the experimental curve and the theoretical curve calculated using intraband optical scattering as the only scattering mechanism could be due to the use of the relaxation time approximation. Since alloy scattering is not present, space-charge scattering was included as a possibility. Curve 2 of figure 6.15 fits the experimental curve with the parameter $N_s Q_s$ in equation 4.43 equal to $0.1 \times 10^6 \text{ m}^{-1}$. This corresponds to a very small density of inhomogeneities;

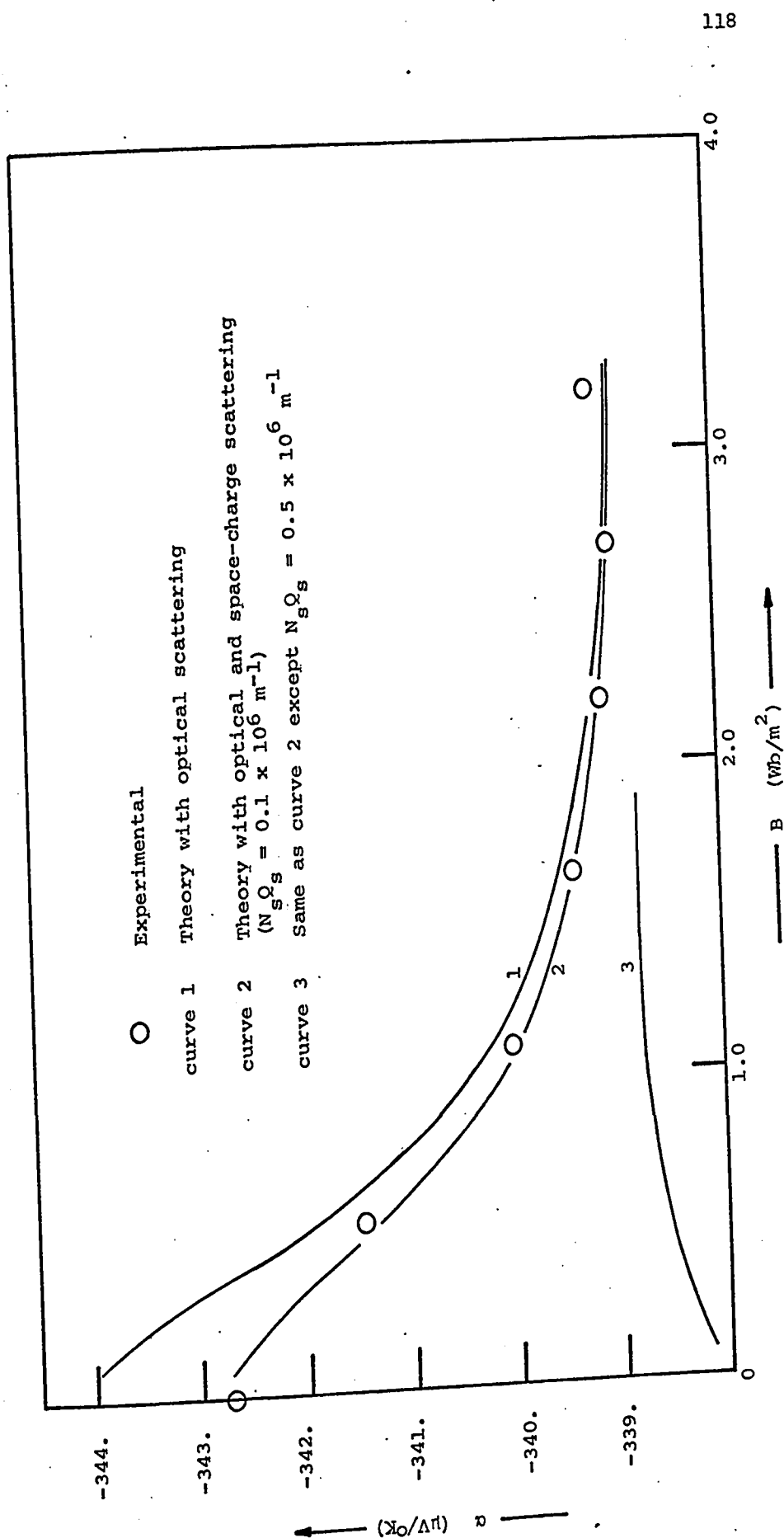


Figure 6.15 Fit to the magneto-Seebeck effect using specific relaxation times, for InAs ($n = 2.92 \times 10^{16} \text{ /cc}$)

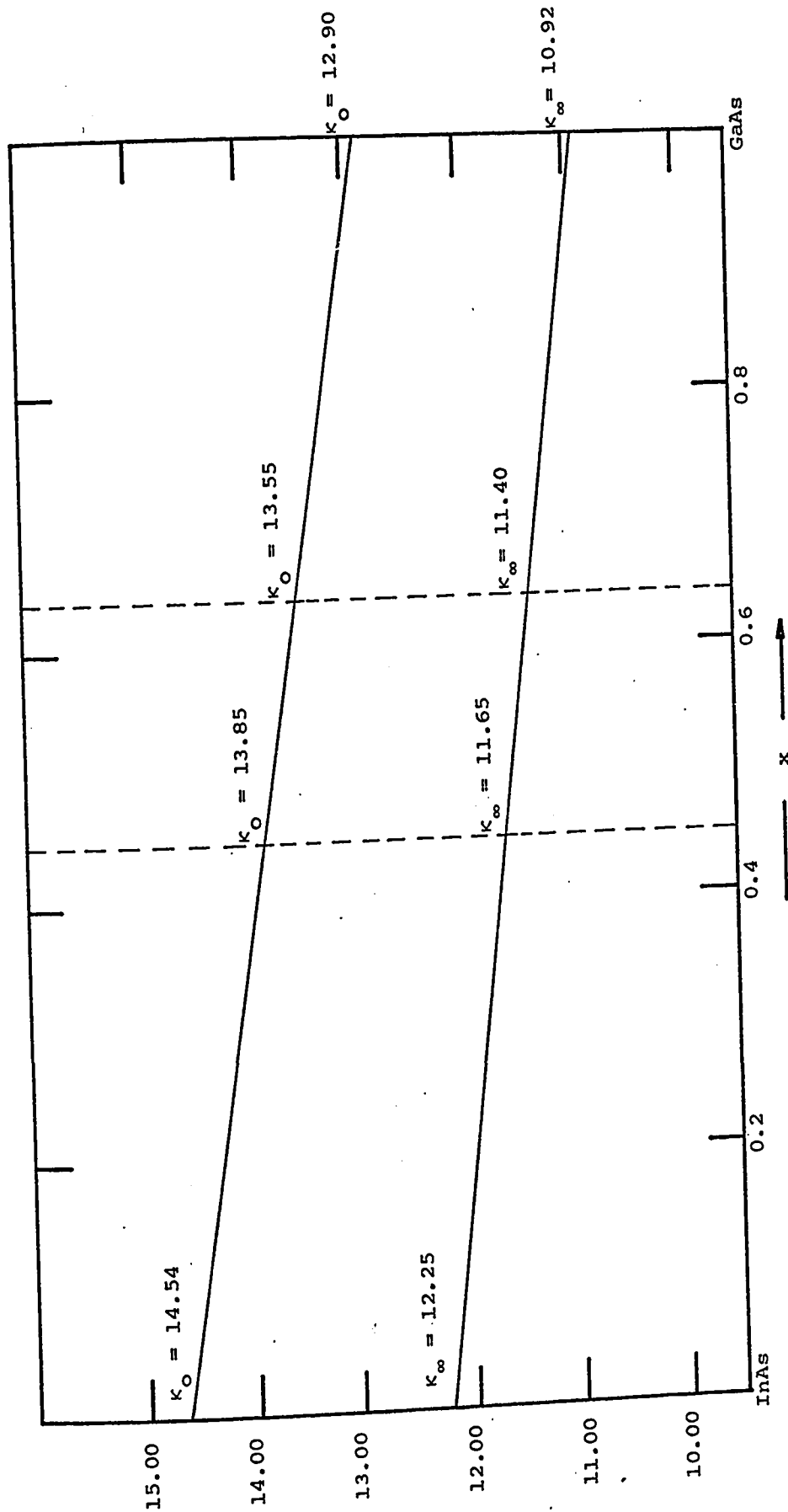


Figure 6.16 Chosen values for the low and high frequency dielectric constants

the usual value of N_{S-Q_S} for compensated material is of the order of $4-5 \times 10^6 \text{ m}^{-1}$. Curve 3 of the same figure shows the strong sensitivity of α vs B to a change in N_{S-Q_S} .

In order to fit the samples in the alloy range, the same parameters were needed for τ_{po} . The optical phonon energy $\hbar\omega_2$ was taken from the same source as for InAs, (70L1). The dielectric constants were linearly interpolated between InAs and GaAs as shown on figure 6.16; the values for GaAs being also taken from Rode (70R1).

Figure 6.17 gives the results for $x = 0.640$. Curve 1 is the theoretical curve with optical phonon and alloy scattering. The number of lattice points N_a , to be included in the constant for alloy scattering, equation 4.49, was calculated in the following way: for $x = 0.640$, the volume of the unit cell is $(5.80 \text{ \AA})^3$ (58W1) and it contains a total of 8 atoms; the total number of atoms per unit volume is therefore $4.1 \times 10^{22}/\text{cc}$. Tietjen and Weisberg (65T1) took an average of the values used by previous workers, $2.6 \times 10^{22}/\text{cc}$, which they included in their calculations of the mobility due to alloy scattering. In this case, the factor C in equation 4.49 was used as an adjustable parameter; the value which provided with a good fit is included in table 6.8.

Curve 2 of figure 6.17 is a similar fit except that alloy scattering is replaced by space-charge scattering. A value of $3.7 \times 10^6 \text{ m}^{-1}$ was needed for N_{S-Q_S} in order to obtain a good fit.

The individual contributions to α vs B from optical phonon scattering and from alloy or space-charge scattering are shown on figure 6.18.

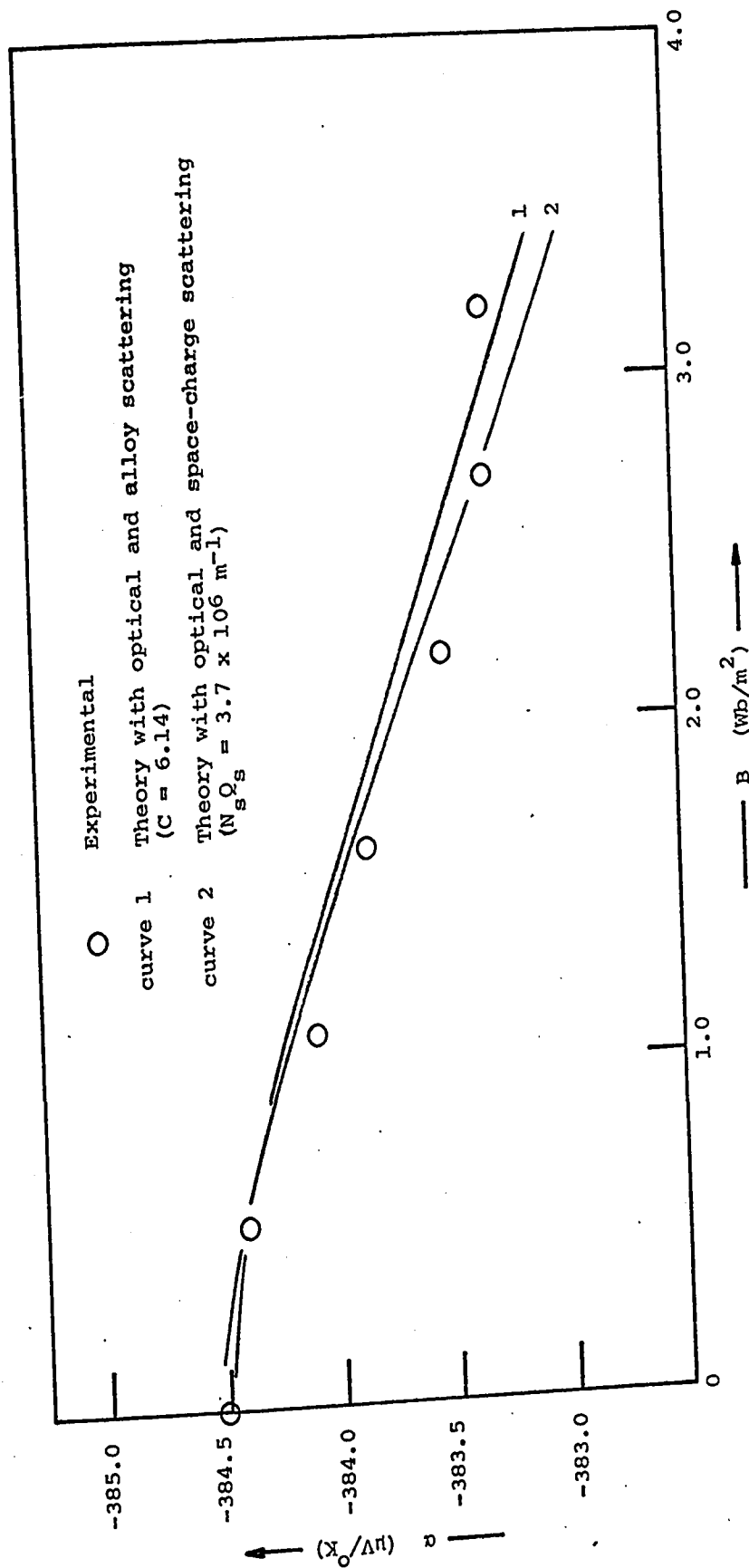


Figure 6.17 Fit to the magneto-Seebeck effect using specific relaxation times, for $x = 0.640$

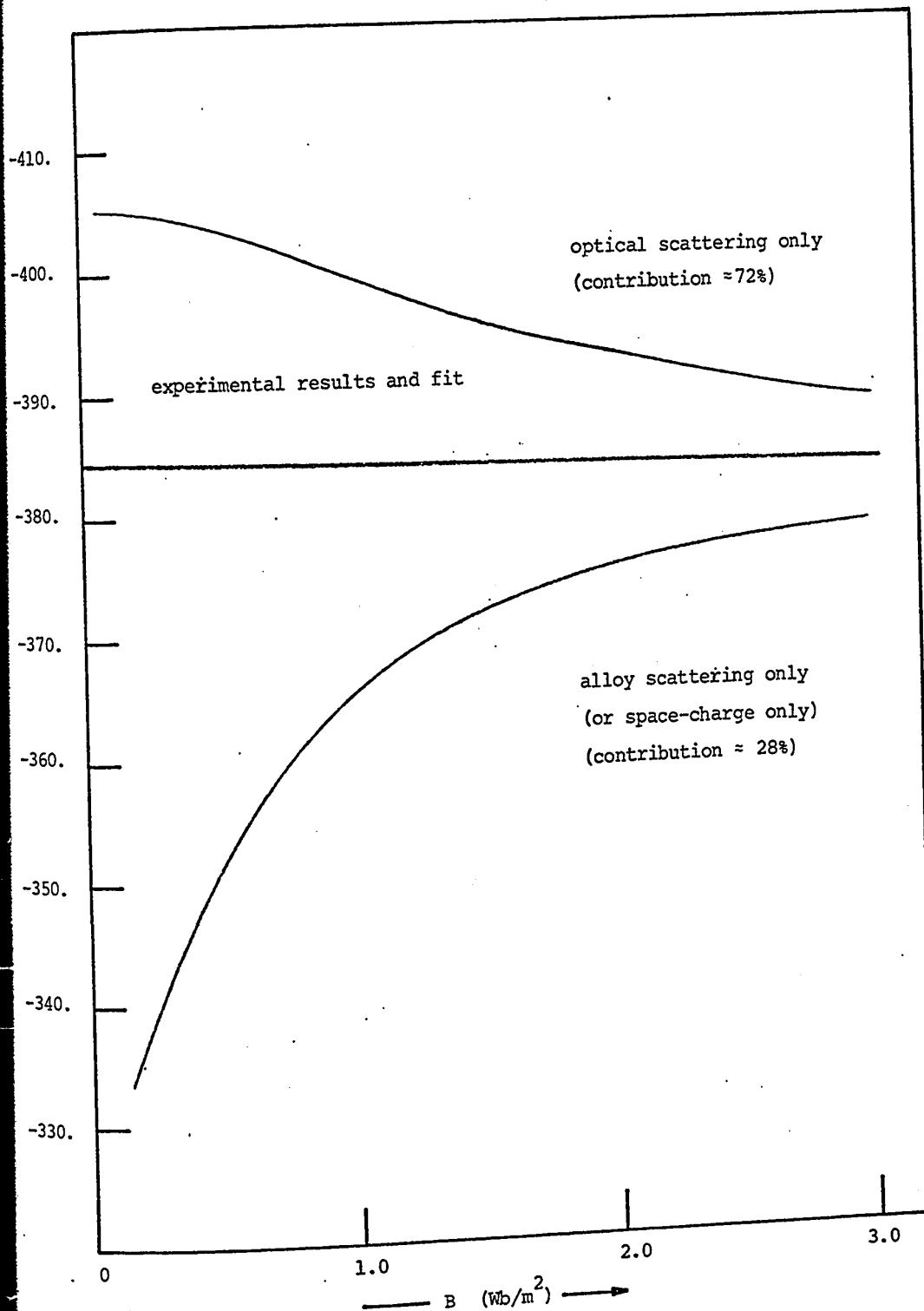


Figure 6.18 Individual contributions to α vs B from each scattering mechanism, for $x = 0.640$

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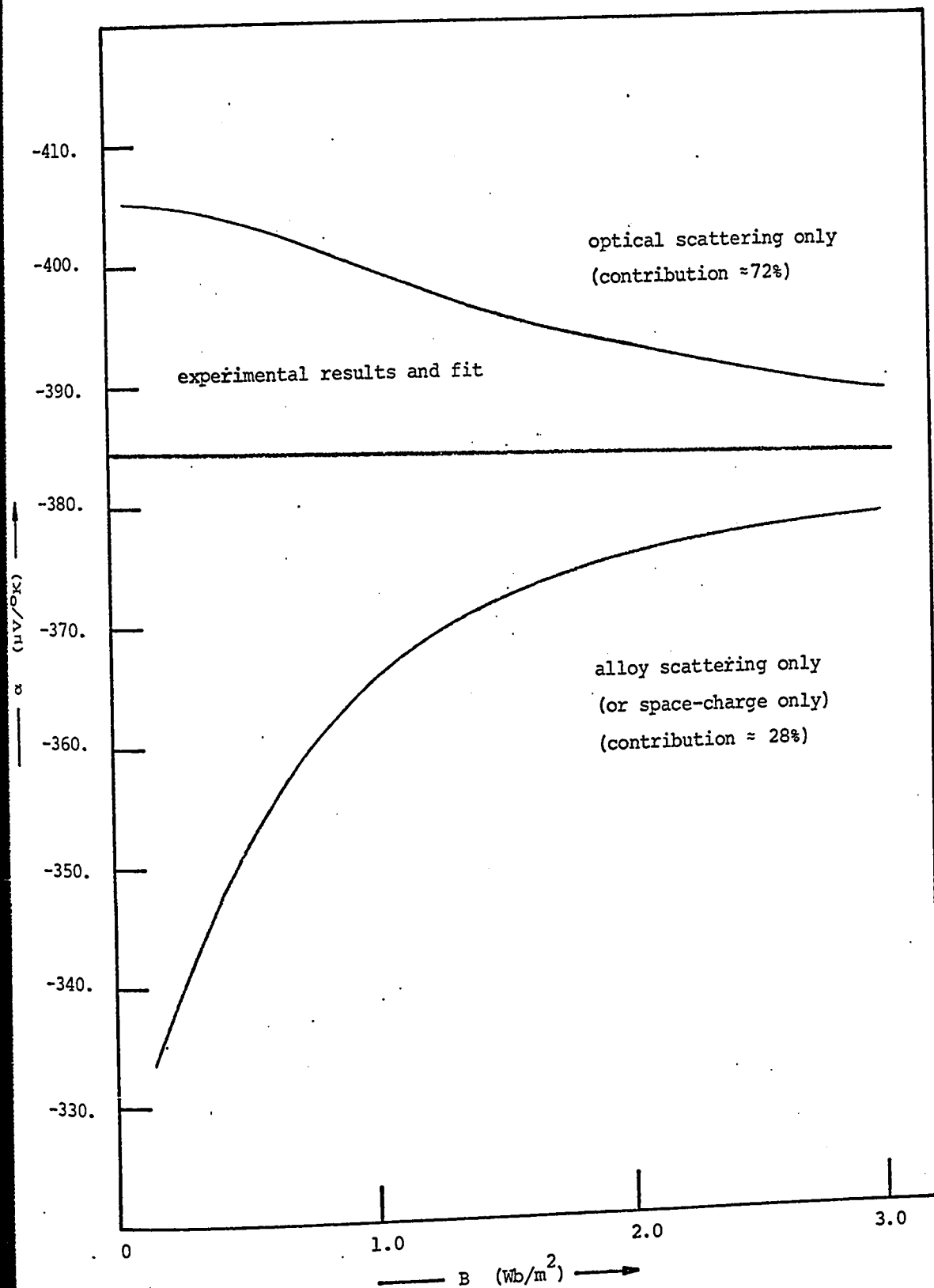


Figure 6.18 Individual contributions to α vs B from each scattering mechanism, for $x = 0.640$

Similar results obtained for $x = 0.450$ are given in figures 6.19 and 6.20, with the adjustable parameters ($N_s Q_s$) or C included in table 6.8.

In order to calculate the percentage contribution of the individual scattering mechanisms to the resultant scattering, the mobilities have been calculated and are listed in table 6.9 for the 3 samples studied in this section. It is shown that the maximum contribution from either of alloy or space-charge scattering in this alloy system is $\approx 28\%$. The contribution reduces as one tends to the individual compounds.

The effective scattering index has been calculated using relation 6.28 and the results are seen in table 6.9, to compare well with the values of s calculated in section 6.3.1. from $\alpha(o)$.

The longitudinal N.-E. coefficients, in the cases when the analysis included only optical scattering or only alloy scattering, were shown on figures 6.18 and 6.20. It is obvious from those curves that the individual coefficients are not simply additive. The resultant coefficients have been calculated using equation 6.29 and the results are given in table 6.9 and compare favourably with the values calculated on the basis of equation 6.26.

From this brief analysis, it is concluded that optical phonons are mainly responsible for scattering in this alloy system.

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In the center of the alloy range, either of alloy or space-charge scattering are plausible as a second scattering mechanism. The adjustable parameters ($N_s Q_s$) and C do not permit a final conclusion to be made on the choice of only one of alloy or space-charge scattering.

It is also concluded on the basis of the results shown in table 6.9, that relations 6.28 and 6.29 can be used to a fairly good approximation.

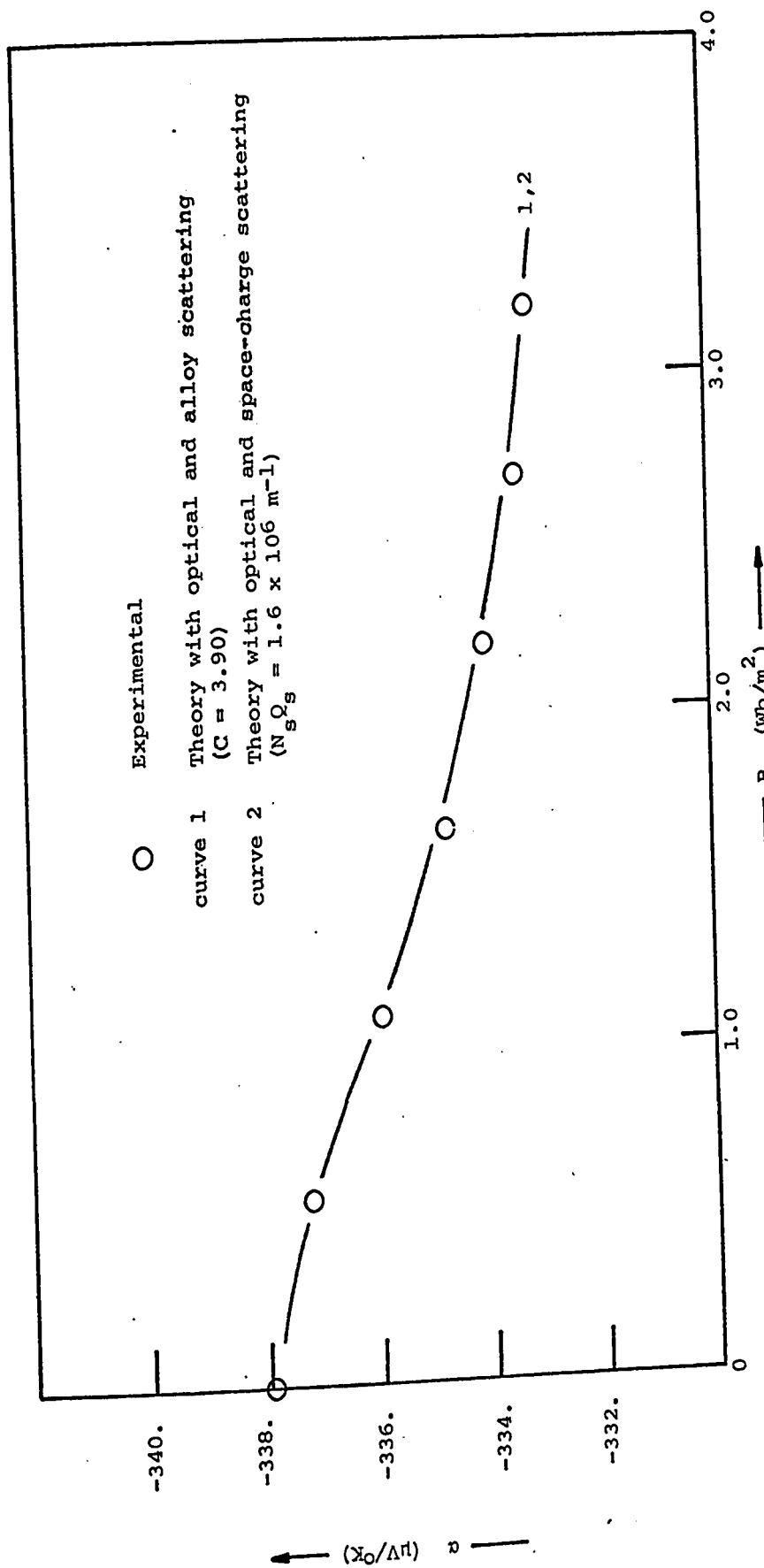


Figure 6.19 Fit to the magneto-Seebeck effect using specific relaxation times, for $x = 0.450$

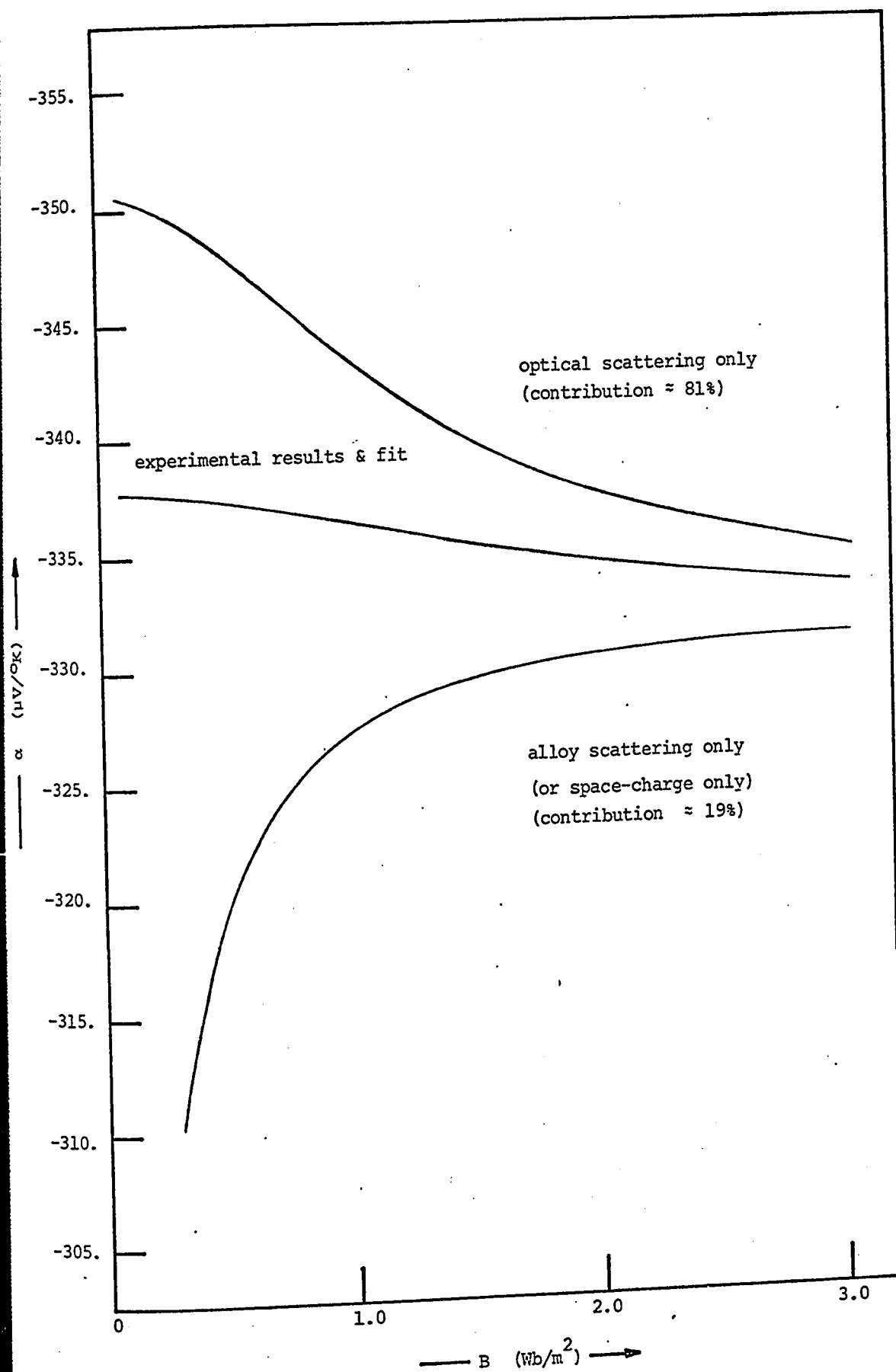


Figure 6.20 Individual contributions to α vs B from each scattering mechanism, for $x = 0.450$

TABLE 6.8

Room temperature parameters providing fits.

MATERIAL PARAMETERS	InAs	x = 0.450	x = 0.640	GaAs
E_o^*	0.397 eV	0.752 eV	0.953 eV	
m_o^*/m	0.023	0.0405	0.0538	
ζ	-1.082	-1.095	-1.76	
$\hbar\omega_l$	0.0301 eV	0.0316 eV	0.0325 eV	
κ_o	14.54	13.85	13.55	
κ_∞	12.25	11.65	11.40	
$(N_{s^+}O_s^-)$ (variable)	$0.1 \times 10^6 \text{ m}^{-1}$	$1.6 \times 10^6 \text{ m}^{-1}$	$3.7 \times 10^6 \text{ m}^{-1}$	
E_i	$E_2 = 0.343 \text{ eV}$			$E_1 = 1.370 \text{ eV}$
N_a		$3.94 \times 10^{22}/\text{cc}$	$4.10 \times 10^{22}/\text{cc}$	
C (variable)		3.90	6.14	

TABLE 6.9

Calculated mobilities and ratios; effective scattering parameters and longitudinal N.-E. coefficients.

CALCULATED	InAs	x = .450	x = .640
μ_1 ($\text{cm}^2/\text{V}\cdot\text{sec}$)	20,190	8,974	6,003
μ_2 ($\text{cm}^2/\text{V}\cdot\text{sec}$)	820,310	39,074	15,137
$\mu = 1/(1/\mu_1 + 1/\mu_2)$ ($\text{cm}^2/\text{V}\cdot\text{s}$)	19,704	7,298	4,298
μ/μ_1	0.976	0.813	0.716
μ/μ_2	0.024	0.187	0.284
$s_{\text{effective}} = s_1 (\mu/\mu_1) + s_2 (\mu/\mu_2)$	.48	.31	.22
s (from $\alpha(0)$, section 6.3.1.)	.48	.32	.23
$\Delta\alpha_1$ ($\mu\text{V}/^\circ\text{K}$)	- 5.2	-16.9	-18.7
$\Delta\alpha_2$ ($\mu\text{V}/^\circ\text{K}$)	+50.0	+46.0	+44.1
$\Delta\alpha$ ($\mu\text{V}/^\circ\text{K}$)	- 3.9	- 5.2	- 1.9
$\Delta\alpha = \frac{\mu}{\mu_1} \Delta\alpha_1 + \frac{\mu}{\mu_2} \Delta\alpha_2$ ($\mu\text{V}/^\circ\text{K}$)	- 3.9	- 5.0	- 0.8

Subscript 1 denotes an analysis including only optical phonon scattering.
 Subscript 2 denotes an analysis including only space-charge scattering.
 No subscript, except when otherwise specified, is a calculation including optical phonon and space-charge scattering (or alloy scattering).

CHAPTER 7

GALLIUM ANTIMONIDE

7.1. INTRODUCTION

The thermomagnetic effects which we are dealing with here have been thoroughly studied and analyzed in chapter 6 in the case of single band effects. It is the author's interest to study the case of two band conduction. As far as the author knows, an application of the formulae for such a case has not been carried out previously.

From the point of view of conduction by two types of carriers, n-type GaSb is particularly interesting. It is well established that the main energy minimum of the conduction band is situated at the center of the Brillouin zone, (Γ_{1c}), (59Z1); this (ooo) band is called the light electron band. The first higher minima are located at the zone boundaries in the $\langle 111 \rangle$ directions, (L_{1c}), at 0.087 eV above the Γ_{1c} minimum (72B1), at room temperature. Already, at relatively low electron concentrations, the $\langle 111 \rangle$ band begins to be populated. The feature of GaSb which draws one's attention, is that although the heavy electrons have a much lower mobility than the light electrons, they contribute significantly to the transport effects in samples with a total carrier concentration

greater than 10^{18} per cm³.

The transport phenomena in n-type GaSb have been investigated by many authors; however, very few used the thermomagnetic effects for a verification or determination of the parameters of the double conduction band or for a study of the electron scattering mechanisms. Such a recent investigation has been presented by Parfenev et al (70Pl); they applied to this material a method proposed by Lang, Pavlov and Parfenev (69Ll). These authors have derived relationships for the magnetothermoelectric power and the transverse N.-E. coefficient for a semiconductor with two types of carriers of the same sign; the relationships are only for the case of strong degeneracy and for weak, intermediate and strong fields. They are only valid for a parabolic band, assuming $\tau_i(E) \propto E^{5/2}$. This assumption has the advantage that all the tensors reduce to a form by which they can be easily calculated.

A method is described here, and applied to GaSb, for using the magneto-Seebeck and transverse N.-E. effects in the case of two types of carriers, for any position of the Fermi level and taking into account the non-parabolicity in the band structure, assuming a band model of the Kane type.

The results of the measurements of the magneto-Seebeck and of the transverse N.-E. effects on a sample of GaSb, are shown on figures 7.1 and 7.3 respectively. The different parameters describing this GaSb sample can be found in section 7.3.

7.2. THEORY AS APPLIED TO GaSb

7.2.1. Magneto-Seebeck effect

Expanding equation 4.1, one obtains:

$$\alpha = \frac{\sum_i \sigma_{11}^i \sum_i \theta_{11}^i - \sum_i \sigma_{11}^i \sum_i \frac{(E_F)}{e_i T} \sigma_{11}^i + \sum_i \sigma_{12}^i \theta_{12}^i - \sum_i \sigma_{12}^i \sum_i \frac{(E_F)}{e_i T} \sigma_{12}^i}{\left[\sum_i \sigma_{11}^i \right]^2 + \left[\sum_i \sigma_{12}^i \right]^2} \quad 7.1$$

In considering carrier transport occurring in many bands simultaneously, the respective tensors given by equations 4.2 have to be added together. This means that if for example, as in GaSb, conduction occurs in the $\langle 111 \rangle$ band where the multiplicity is M , this has to be included explicitly.

Considering the multiplicity of the (ooo) band as one and that of the $\langle 111 \rangle$ band as M , one obtains for such a case:

$$\alpha = \frac{(\sigma_{11}^1 + M\sigma_{11}^2)(\theta_{11}^1 + M\theta_{11}^2) - (\sigma_{11}^1 + M\sigma_{11}^2) \left[\frac{E_F}{e_1^T} \frac{1}{11} \sigma_{11}^1 + \frac{E_F}{e_2^T} \frac{2}{11} M\sigma_{11}^2 \right] + (\sigma_{12}^1 + M\sigma_{12}^2)(\theta_{12}^1 + M\theta_{12}^2) - (\sigma_{12}^1 + M\sigma_{12}^2) \left[\frac{E_F}{e_1^T} \frac{1}{12} \sigma_{12}^1 + \frac{E_F}{e_2^T} \frac{2}{12} M\sigma_{12}^2 \right]}{(\sigma_{11}^1 + M\sigma_{11}^2)^2 + (\sigma_{12}^1 + M\sigma_{12}^2)^2} \quad 7.2$$

Rearranging:

$$\alpha = \frac{(\sigma_{11}^1 + M\sigma_{11}^2)(\theta_{11}^1 + M\theta_{11}^2) + (\sigma_{12}^1 + M\sigma_{12}^2)(\theta_{12}^1 + M\theta_{12}^2) - \frac{E_F}{e_1^T} \left[\sigma_{11}^1 (\sigma_{11}^1 + M\sigma_{11}^2) + \sigma_{12}^1 (\sigma_{12}^1 + M\sigma_{12}^2) \right] - \frac{E_F}{e_2^T} \left[M\sigma_{11}^2 (\sigma_{11}^1 + M\sigma_{11}^2) + M\sigma_{12}^2 (\sigma_{12}^1 + M\sigma_{12}^2) \right]}{(\sigma_{11}^1 + M\sigma_{11}^2)^2 + (\sigma_{12}^1 + M\sigma_{12}^2)^2} \quad 7$$

In order to simplify the previous equations, the following terminology is adopted:

Let

$$\begin{array}{ll} \sigma_{11}^1 \equiv B_3 & M\sigma_{11}^2 \equiv B_4 \\ \sigma_{12}^1 \equiv B_1 & M\sigma_{12}^2 \equiv B_2 \\ \theta_{11}^1 \equiv B_5 & M\theta_{11}^2 \equiv B_6 \\ \theta_{12}^1 \equiv B_7 & M\theta_{12}^2 \equiv B_8 \end{array}$$

Where each B_i represents an individual integration.

Also, let:

$$G_1 = B_3 + B_4$$

$$G_2 = B_1 + B_2$$

The magneto-Seebeck effect then becomes:

$$\alpha = \frac{G_1 (B_5 + B_6) + G_2 (B_7 + B_8) - \frac{(E_F)}{e_1 T} [B_3 G_1 + B_1 G_2] - \frac{(E_F)}{e_2 T} [B_4 G_1 + B_2 G_2]}{G_1^2 + G_2^2} \quad 7.4$$

Valid for carrier transport in 2 bands with e_i being either of $\pm e$.

The tensors to be included in equation 7.4 are:

$$\begin{aligned}
 B_1 &\equiv \sigma_{12}^1 = \frac{e_1 B}{3\pi^2} \int_0^\infty \left(-\frac{\partial f_0}{\partial \xi}\right)_1 \mu_1 c_1 k_1^3 d\xi_1 \\
 B_2 &\equiv M\sigma_{12}^2 = M \frac{e_2 B}{3\pi^2} \int_0^\infty \left(-\frac{\partial f_0}{\partial \xi}\right)_2 \mu_2 c_2 k_2^3 d\xi_2 \\
 B_3 &\equiv \sigma_{11}^1 = \frac{e_1}{3\pi^2} \int_0^\infty \left(-\frac{\partial f_0}{\partial \xi}\right)_1 c_1 k_1^3 d\xi_1 \\
 B_4 &\equiv M\sigma_{11}^2 = M \frac{e_2}{3\pi^2} \int_0^\infty \left(-\frac{\partial f_0}{\partial \xi}\right)_2 c_2 k_2^3 d\xi_2 \\
 B_5 &\equiv \theta_{11}^1 = \frac{k}{3\pi^2} \int_0^\infty \left(-\frac{\partial f_0}{\partial \xi}\right)_1 \xi_1 c_1 k_1^3 d\xi_1 \\
 B_6 &\equiv M\theta_{11}^2 = M \frac{k}{3\pi^2} \int_0^\infty \left(-\frac{\partial f_0}{\partial \xi}\right)_2 \xi_2 c_2 k_2^3 d\xi_2 \\
 B_7 &\equiv \theta_{12}^1 = \frac{kB}{3\pi^2} \int_0^\infty \left(-\frac{\partial f_0}{\partial \xi}\right)_1 \xi_1 \mu_1 c_1 k_1^3 d\xi_1 \\
 B_8 &\equiv M\theta_{12}^2 = M \frac{kB}{3\pi^2} \int_0^\infty \left(-\frac{\partial f_0}{\partial \xi}\right)_2 \xi_2 \mu_2 c_2 k_2^3 d\xi_2
 \end{aligned}$$

7.5

where

$$c_i = \frac{\mu_i}{1 + \mu_i^2 B^2}$$

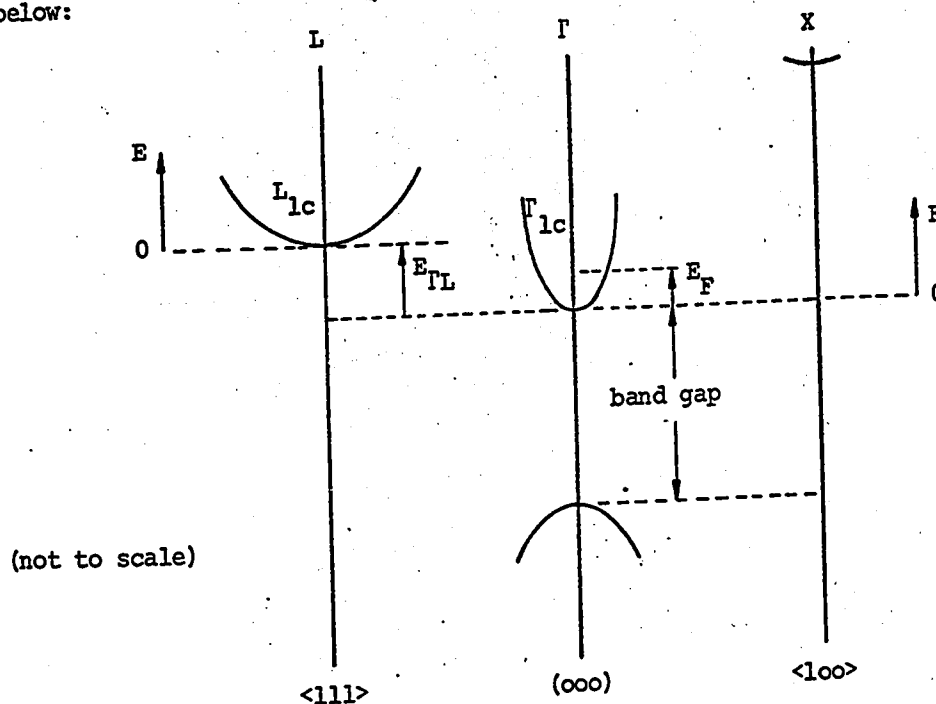
7.6

It becomes obvious from equations 7.4 and 7.5 that in order to calculate α , one has to adopt definitions for the following:

$$e_i, M, (E_F)_i.$$

Since the measurements were made on n-type GaSb with a total carrier concentration large enough to populate the $\langle 111 \rangle$ band, $e_1 = e_2 = -e$.

The band structure of GaSb is, qualitatively, as shown below:



To simplify the numerical integrations, the Fermi energies $(E_F)_i$ corresponding to each band will be defined by considering the bottom of each of the Γ_{1c} and L_{1c} bands as having a value of energy equal to zero.

The Fermi energies are therefore:

$$(E_F)_1 = E_F$$

and

$$(E_F)_2 = -(E_{TL} - E_F)$$

The final expression for the thermoelectric power in a transverse magnetic field is:

$$\alpha = \frac{G_1(B_5+B_6) + G_2(B_7+B_8) + \frac{k}{e} \zeta [B_3 G_1 + B_1 G_2] + \frac{k}{e} (\zeta - \frac{E_{TL}}{kT}) [B_4 G_1 + B_2 G_2]}{G_1^2 + G_2^2} \quad 7.8$$

7.2.2. Transverse N.-E. effect

Using a similar treatment as for α , this coefficient becomes, after rearranging equation 4.9,

$$\begin{aligned} Q_1 = \frac{1}{B} & \frac{(\sigma_{12}^1 + M\sigma_{12}^2)(\theta_{11}^1 + M\theta_{11}^2) - (\sigma_{11}^1 + M\sigma_{11}^2)(\theta_{12}^1 + M\theta_{12}^2) + M\sigma_{11}^2\sigma_{12}^1 \left[\frac{(E_F)_1}{e_1^T} - \frac{(E_F)_2}{e_2^T} \right]}{(\sigma_{11}^1 + M\sigma_{11}^2)^2 + (\sigma_{12}^1 + M\sigma_{12}^2)^2} \\ & + \frac{\sigma_{11}^1 M\sigma_{12}^2 \left[\frac{(E_F)_2}{e_2^T} - \frac{(E_F)_1}{e_1^T} \right]}{(\sigma_{11}^1 + M\sigma_{11}^2)^2 + (\sigma_{12}^1 + M\sigma_{12}^2)^2} \quad 7.9 \end{aligned}$$

With the same convention for e_i and $(E_F)_i$:

$$Q_1 = \frac{1}{B} \frac{(\quad)(\quad) - (\quad)(\quad) + \frac{E_{FL}}{eT} [\sigma_{11}^1 \sigma_{12}^2 - \sigma_{11}^2 \sigma_{12}^1]}{(\quad)^2 + (\quad)^2} \quad 7.10$$

Applying the terminology described by equations 7.5,

$$Q_1 = \frac{1}{B} \frac{G_2(B_5 + B_6) - G_1(B_7 + B_8) + \frac{E_{FL}}{eT} (B_2 B_3 - B_1 B_4)}{G_1^2 + G_2^2} \quad 7.11$$

For the case of one carrier, n-type, equations 7.8 and

7.11 will reduce to:

$$\alpha = \frac{B_3 B_5 + B_1 B_7 + \frac{E_F}{eT} (B_3^2 + B_1^2)}{B_3^2 + B_1^2} \quad 7.12$$

and

$$Q_1 = \frac{1}{B} \frac{B_1 B_5 - B_3 B_7}{B_3^2 + B_1^2} \quad 7.13$$

Equations 7.12 and 7.13 can be compared with equations 6.1 and 6.8; equations 7.12 and 7.13 are easier to use in computations, if the conventions, described in this chapter, are adopted.

7.3. CHOICE OF PARAMETERS

In order to calculate theoretically the values of α and Q_1 according to equations 7.8 and 7.11, various parameters are needed:

E_o^* : effective mass band gap,

m_{01}^* : bottom of the band effective mass for the
(ooo) band,

m_2^* : effective mass for the $\langle 111 \rangle$ band,

E_{FL} and E_F .

These parameters were chosen as:

Band gap.

$$E_{oo} = 0.813 \text{ eV} \quad (59Z1)$$

$$E_o = E_{oo} + \frac{\alpha T^2}{\theta + T} \quad (67V1)$$

with $\alpha = -5.4 \times 10^{-4} \text{ eV/}^\circ\text{K} \quad (61W1)$

$$\theta = 112.4 \text{ }^\circ\text{K}$$

Effective masses.

$$m_{01}^* (0^\circ\text{K}) = 0.042m \quad (70H1)$$

$$m_2^* (\text{room temperature}) = 0.226m \quad (69T1)$$

with an ellipticity parameter

K of 8.6

(64P1)

The measurements of α and Q_1 were made on a sample of GaSb on which previous high temperature transport measurements had been made in this laboratory. These measurements of resistivity and Hall coefficient as a function of magnetic field and temperature have been analyzed and published by Basinski, Kwan and Woolley (72B1). The following parameters were determined:

$$\text{a) } E_{\Gamma_L}(o) = 0.097 \text{ eV with a temperature coefficient of } -3.4 \times 10^{-5} \text{ eV/}^\circ\text{K.}$$

$$\begin{aligned} \text{b) } n_1 &= 3.757 \times 10^{17} / \text{cc}, & \mu_1 &= 3.760 \times 10^3 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1} \\ n_2 &= 1.07 \times 10^{18} / \text{cc}, & \mu_2 &= 4.91 \times 10^2 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1} \end{aligned}$$

$$\text{c) } E_F = +0.0292 \text{ eV}$$

7.4. ANALYSIS, RESULTS AND DISCUSSION

7.4.1. STUDY OF THE SCATTERING USING TWO SCATTERING PARAMETERS,

$$\underline{s_1 \text{ FOR BAND (000) AND } s_2 \text{ FOR BAND } \langle 111 \rangle}$$

7.4.1.1. Method of Analysis

An attempt was made initially, to fit the experimental curve of α vs B using, for the relaxation time of each type of electron, the

"generalized form":

$$\tau_i = (\tau_o)_i k_i^{2s_i-1} \left(\frac{dE}{dk}\right)_i \quad 7.14$$

The only unknown parameters to fit with, are s_1 and s_2 .

All the other needed parameters, E_o^* , m_{o1}^* , m_2^* , σ_1 , σ_2 , E_{TL} and E_F are considered as fixed constants.

Note:

Refer to Appendix 6.1 for a description of how $(\tau_o)_i$ is calculated using σ_i .

7.4.1.2. Results and discussion

Figure 7.1 shows the variation of the thermoelectric power with the magnetic field induction B. The fit was only possible with values of $s_1 = -0.26$ and $s_2 = -0.36$; the absolute value of α is, percentage wise, in good agreement with the experimental curve.

The longitudinal N.-E. coefficient is displayed on figure 7.2 where the overall shape of the curve can be studied more closely.

The transverse N.-E. coefficient, figure 7.3, is lower in value than the experimental curve. Note that the theoretical curve is calculated using the values of s_1 and s_2 which gave the best possible fit to α vs B. It was shown in the previous chapter, for the alloy system of $Ga_x In_{1-x} As$, that it was possible to fit the measured coefficient of this effect only if a constant $\overline{Q}_1(i)$ was added to the theoretically

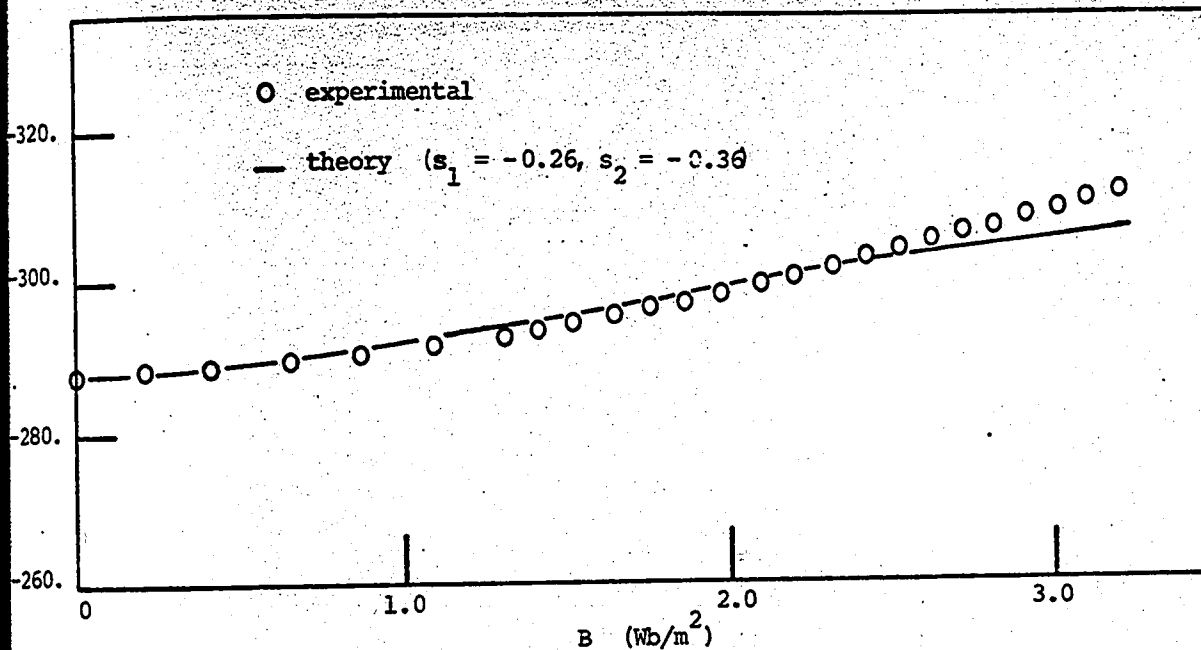


Figure 7.1 Magneto-Seebeck coefficient for GaSb and fit using s_1 and s_2

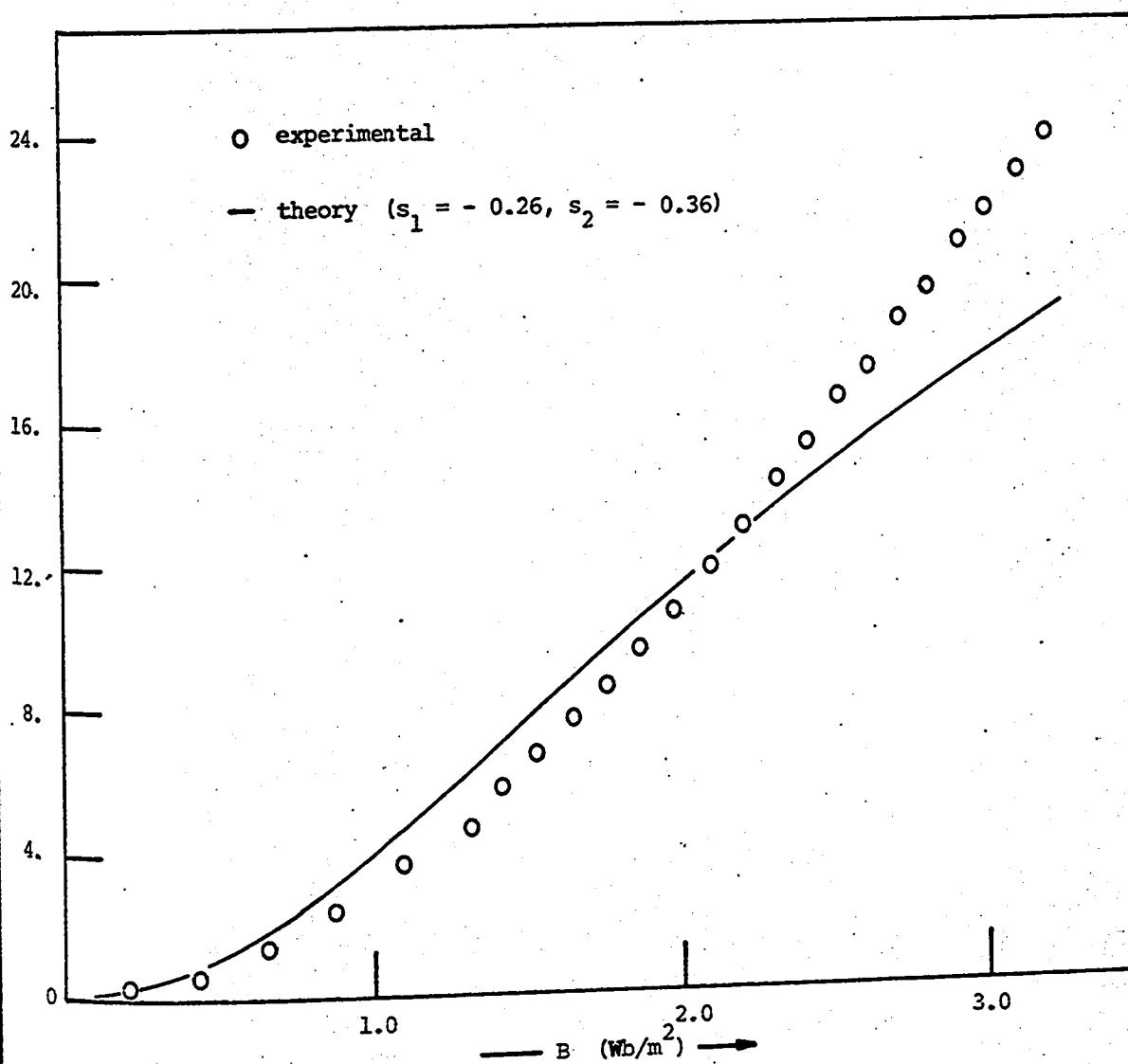


Figure 7.2 Longitudinal N.-E. coefficient for GaSb and fit using s_1 and s_2

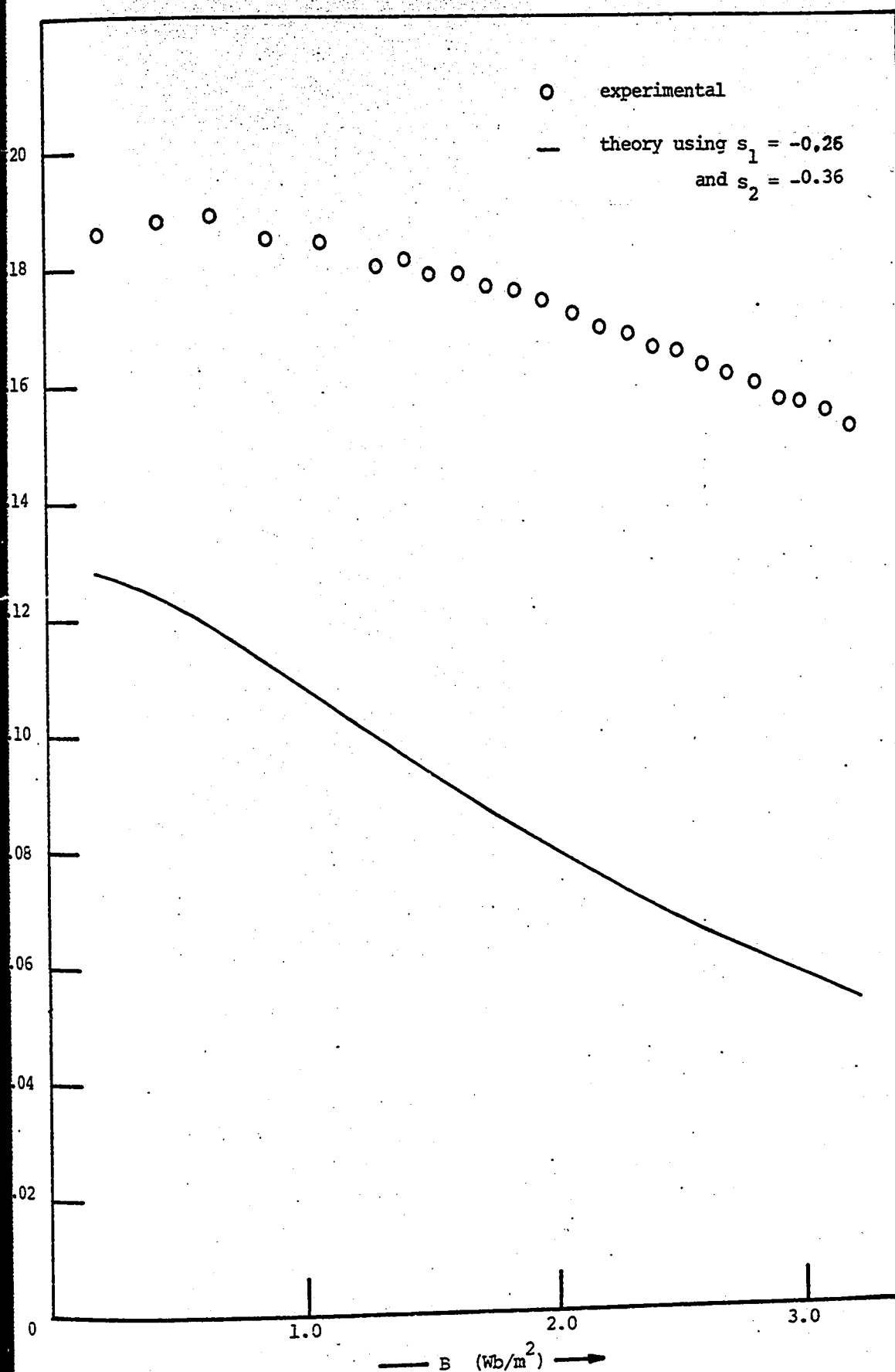


Figure 7.3 Transverse N.-E. coefficient for GaSb and theory using s_1 and s_2

calculated values. $Q_1(i)$ is the contribution from the inhomogeneities. Therefore, one may expect in the work on GaSb, that the transverse N.-E. coefficient will here also, be affected to some extent by the presence of inhomogeneities.

On that basis, the difference between the curves on figure 7.3 is partially attributed to the presence of inhomogeneities.

It was mentioned in chapter 6, that the relaxation time described by equation 7.14 has a limited validity of application. Non-parabolicity effects are not taken into account in the scattering probability. This is discussed extensively by Zawadzki and Szymanska (71Z1); this paper also shows that considering $(\tau_o)_i$ as a constant is not always valid. For example, in the presence of scattering by charged centers, the effect of screening leads to an energy dependence which should be incorporated in $(\tau_o)_i$. This usual procedure of neglecting the energy dependence due to screening produces an overestimation of this mode in the thermomagnetic effects. This conclusion is in agreement with the results shown on figures 7.2 and 7.3 where $\Delta\alpha$ and Q_1 (theory) are both smaller in value as compared with the experimental results.

This method of analysis has, however, the important usefulness that in some cases it may provide an insight on the possible scattering mechanisms present in a semiconductor. This is even more true, at low carrier concentrations, in single band semiconductors where the possibility of s being an "effective" scattering parameter, representing a combination of many scattering mechanisms, is much more limited.

From the results of $s_2 = -0.36$, it seems clear that acoustic scattering is present in the $\langle 111 \rangle$ band. Since the carrier concentration is relatively high, ionized impurity scattering is probably also effective.

As for $s_1 = -0.26$, considering the work done by other authors, for example on GaAs, the presence of optical phonon and ionized impurity scattering seems reasonable; the negative sign of s_1 can be explained by the presence of compensated regions in the material, since space-charge scattering has a parameter of $-\frac{1}{2}$. Because of the presence of the $\langle 111 \rangle$ band at a distance of only 0.087 eV, interband scattering may also be a possibility. The extent to which either of these mechanisms are present cannot be determined from the present analysis.

7.4.2. STUDY OF THE SCATTERING USING CHOSEN RELAXATION TIMES

7.4.2.1. Analysis and chosen parameters

The magnetic field dependence of the magneto-Seebeck and transverse N.-E. coefficients will be calculated for a mixed scattering mechanism and compared with the experimental results.

The relaxation time will be defined by the following equation instead of equation 7.14 used in the previous analysis:

$$\frac{1}{\tau} = \sum_i \frac{1}{\tau_i}$$

The scattering mechanisms chosen, so as to define the relaxation times of the electrons in the two different bands will now be mentioned. The different parameters needed, so as to fully describe each individual scattering mechanism, follow with the associated references.

Γ_{lc} band (spherical, non-parabolic)

- i) Intraband optical phonon scattering, equations 4.29 to 4.32.

$$(\hbar\omega_l)_{\Gamma_{lc}} = 0.0297 \text{ eV} \quad (63M1)$$

$$\kappa_{\infty} = 13.8 \quad (70R1)$$

$$\kappa_0 = 15.0 \quad (70R1)$$

- ii) Interband optical phonon scattering, equation 4.33.

$$\hbar\omega_{12} = 0.8 (\hbar\omega_l)_{\Gamma_{lc}} \quad (63D1, 63M1)$$

$$\rho = 5.6137 \text{ gm/cc} \quad (68M1)$$

$$M = 4 \quad (69P1)$$

$$m_d^* = (m_L^* m_T^*)^{2/3} = m_2^*$$

$$E_{12} = E_{\Gamma_L}$$

$$D_{12} = \text{adjustable}$$

- iii) Acoustic phonon scattering "deformation potential",
equation 4.24.

$$U_2 = 4.298 \times 10^5 \text{ cm/sec} \quad (68M1)$$

$$(E_1)_{\Gamma_{1c}} = 8.0 \text{ eV} \quad (70S1)$$

- iv) Ionized impurity scattering, equations 4.39 and 4.42.

$$(N_I)_{\Gamma_{1c}}, \quad \text{adjustable}$$

- v) Space-charge scattering, equation 4.43.

$$m_o^* = m_{ol}^*$$

$$(N_{S^-})_{S^-}, \quad \text{adjustable}$$

Because of the number of adjustable parameters, it is not possible to obtain a meaningful model from the magnetothermal effects alone since the measurements were made at only one temperature. The transport properties have been analyzed for this GaSb sample (72B1) and curves of mobility versus temperature, one for the Γ_{1c} band and one for the L_{1c} band, have been obtained.

A theoretical curve has been calculated and compared with the experimental results of μ_1 vs T by Basinski et al (72B2).

As for the mobility μ_2 in the L_{1c} band versus temperature, it has been compared, by the present author and J. Basinski (72B4), with results from a model which included the major possible scattering mechanisms for this band.

In order to describe the scattering in the Γ_{1c} band, two theoretical models are suggested (72B2) as possible combinations of the different scattering modes: model a and model b. These models are limiting cases and provide a possible range of values for the different adjustable parameters. Model a includes all the possible scattering modes mentioned above. The adjustable parameters D_{12} , $(N_I)\Gamma_{1c}$ and $N_s Q_s$ are said to give a good fit for the following values:

$$\begin{aligned} D_{12} &= 4.4 \times 10^8 \text{ eV/cm} \\ (N_I)\Gamma_{1c} &= 2.1 \times 10^{18} / \text{cc} \\ \text{and } N_s Q_s &= 2.9 \times 10^6 \text{ m}^{-1} \end{aligned}$$

In this model, $(N_I)\Gamma_{1c}$ was kept constant and the other two parameters were adjusted. In order to obtain a range of possible values for $(N_I)\Gamma_{1c}$, model b did not include space-charge scattering and in that case, D_{12} and $(N_I)\Gamma_{1c}$ were the variables. The results for model b are the following:

$$\begin{aligned} D_{12} &= 3.8 \times 10^8 \text{ eV/cm} \\ \text{and } (N_I)\Gamma_{1c} &= 3.37 \times 10^{18} / \text{cc} \end{aligned}$$

The range of the parameters which obviously do not have unique values is therefore:

$$3.8 \times 10^8 \frac{\text{eV}}{\text{cm}} \leq D_{12} < 4.4 \times 10^8 \text{ eV/cm}$$

$$2.1 \times 10^{18}/\text{cc} \leq (N_I)_{1c} \leq 3.37 \times 10^{18}/\text{cc}$$

$$0 \leq N_{s0s} \leq 2.9 \times 10^6 \text{ m}^{-1}$$

The number of ionized impurities was chosen as $2.1 \times 10^{18}/\text{cc}$ in model a, on account of the following:

In the absence of compensation in an n-type material,

$$N_I = N_D$$

$$\text{and } n = N_D$$

where N_D is the number of donors per unit volume and n is the total carrier concentration.

In GaSb, compensating acceptors are present in all samples; if the acceptors are assumed to be doubly charged (Baxter, Reid and Beer, 67Bl), considering a Z^2 scattering law, each doubly charged center will scatter as effectively as four singly charged centers. Thus, the "effective" density of charged centers will be:

$$N_I = N_D + 4 N_A$$

7.16

where N_A is the number of acceptors.

The carrier concentration will be:

$$n = N_D - 2N_A \quad 7.17$$

One finally obtains for the "effective number of ionized impurities:

$$N_I = n + 6N_A \quad 7.18$$

If N_A is chosen as $1.1 \times 10^{17}/\text{cc}$ (67B1, 72B2), $N_I = 2.1 \times 10^{18}/\text{cc}$. As for the value of $3.37 \times 10^{18}/\text{cc}$ in model b, this is an upper limit for N_I . The total number of scatterers may be increased from 2.1 to $3.37 \times 10^{18}/\text{cc}$ if the heavy electrons of the L_{1c} band are also considered as scattering centers. One obtains in such a case:

$$(N_I)_{\Gamma_{1c}} = n + 6N_A + n_2 \quad 7.19$$

where N_A has a value of $1.4 \times 10^{17}/\text{cc}$.

Since the heavy electrons are in motion, they are unlikely to scatter as efficiently as the ionized impurities; hence, equation 7.19 represents an upper limit for $(N_I)_{\Gamma_{1c}}$.

The analysis of the scattering mechanisms in the $\langle 111 \rangle$ band gave the following results: (Basinski, Demars and Woolley, 72B4)

L_{1c} band (ellipsoidal, parabolic)

- i) Acoustic scattering, equation 4.23.

$$m^* = m_2^*$$

$$(E_1)_{L_{1c}}, \text{ adjustable}$$

- ii) Ionized impurity scattering, equations 4.34 to 4.36.

$$m^* = m_2^*$$

$$(N_I)_{L_{1c}} = 2.3 \times 10^{18}/\text{cc}$$

$$(\text{with } N_A = 1.4 \times 10^{17}/\text{cc})$$

- iii) Intraband polar optical phonon scattering,
equations 4.29 to 4.32.

$$(\hbar\omega_{\ell})_{L_{1c}} = \hbar\omega_{12} = 0.8 (\hbar\omega_{\ell})_{L_{1c}}$$

- iv) Intervalley optical phonon scattering (68Cl).
(Similar to interband scattering, equation 4.33)

$$\frac{1}{\tau_{iv}} = \frac{3}{4} \frac{D_{jj'}^2 (M_d^*)^{3/2}}{\sqrt{2} \pi \hbar^3 \rho \omega_{jj'}} \cdot \frac{1}{e^{x_{jj'}} - 1}$$

$$\cdot [(E + \hbar\omega_{jj'})^{1/2} + e^{x_{jj'}} (E - \hbar\omega_{jj'})^{1/2}] \quad 7.20$$

$$\hbar\omega_{jj'} = (\hbar\omega_g)_{L_{1c}} \quad (66B1)$$

$$x_{jj'} = \hbar\omega_{jj'}/kT$$

$$D_{jj'}, \quad \text{adjustable}$$

The factor 3/4 in the above equation takes account of the fact that transitions between valleys at opposite ends of the same $\langle 111 \rangle$ axis require no phonon at all, while those between valleys on different $\langle 111 \rangle$ axes require the Longitudinal Optical (LO) phonon at the zone edge in the $\langle 111 \rangle$ directions. Hence, three of the ellipsoids are considered from a total of four.

The values of $(E_1)_{L_{1c}}$ and $D_{jj'}$, which provided with the best possible fit to the curve of the mobility μ_2 as a function of temperature are the following:

$$(E_1)_{L_{1c}} = 10 \text{ eV}$$

$$\text{and } D_{jj'} = 7.0 \times 10^8 \text{ eV/cm}$$

7.4.2.2. Results and discussion

The thermomagnetic effects have then been calculated using the above data and the results from model a describing the scattering in the Γ_{1c} band. No adjustable parameters were used. The results obtained and the comparison with the experimental data are shown on figures 7.4 and 7.5. These display respectively the longitudinal and transverse N.-E. coefficients. The percentage

deviations of the calculations with respect to the experimental results are given in Table 7.1. It is seen that the theoretical values of the thermoelectric power and of the transverse N.-E. coefficient are respectively 13% and 3% lower than the experimental values while the longitudinal N.-E. coefficient (at 3.2 Wb/m^2) is 1.7% below the corresponding experimental data.

The author wishes to point out that the deviation is much larger than the possible experimental error in the case of $\alpha(o)$ and comparable in the case of $\Delta\alpha$ and $Q_{\perp}$. Looking at figures 7.4 and 7.5, the scattering of the points can be estimated to be 1-2% in the case of the longitudinal N.-E. coefficient at high fields and also 1-2% in the case of the transverse N.-E. coefficient at low fields. Even if one would consider a systematic error due to the possible imperfect thermal contacts, as discussed in section 5.4.3., the observed deviation in the thermoelectric power could not be explained on this basis.

Furthermore, the experimental values compare well with those obtained by other authors. For example, Silverman, Carlson and Ehrenreich (63S2) measured the Seebeck coefficient and the transverse N.-E. coefficient in n-type GaSb at 300°K . Their results were the following:

	R_o	α_o	$Q_{\perp} (0.6 \text{ Wb/m}^2)$
	cm^3/coul	$\mu\text{V}/^{\circ}\text{K}$	$\text{cm}^2/^{\circ}\text{K sec}$
1	-13	-350	+ 0.16
2	- 9	-288	+ 0.19
3	- 3	-230	+ 0.15

1 and 3 are from (63S2); 2 is the present work.

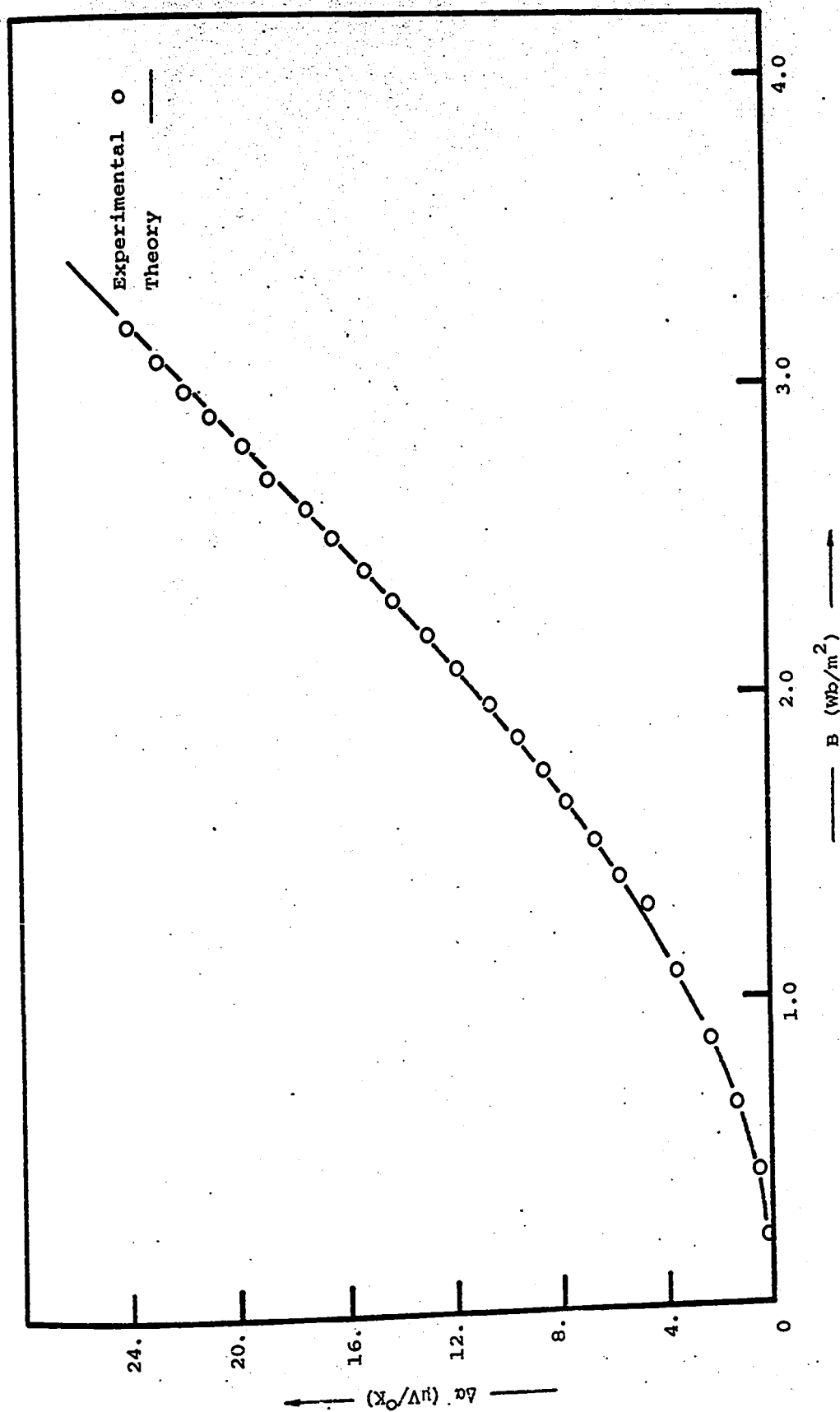


Figure 7.4 Longitudinal N.-E. coefficient for GaSb and fit using specific relaxation times

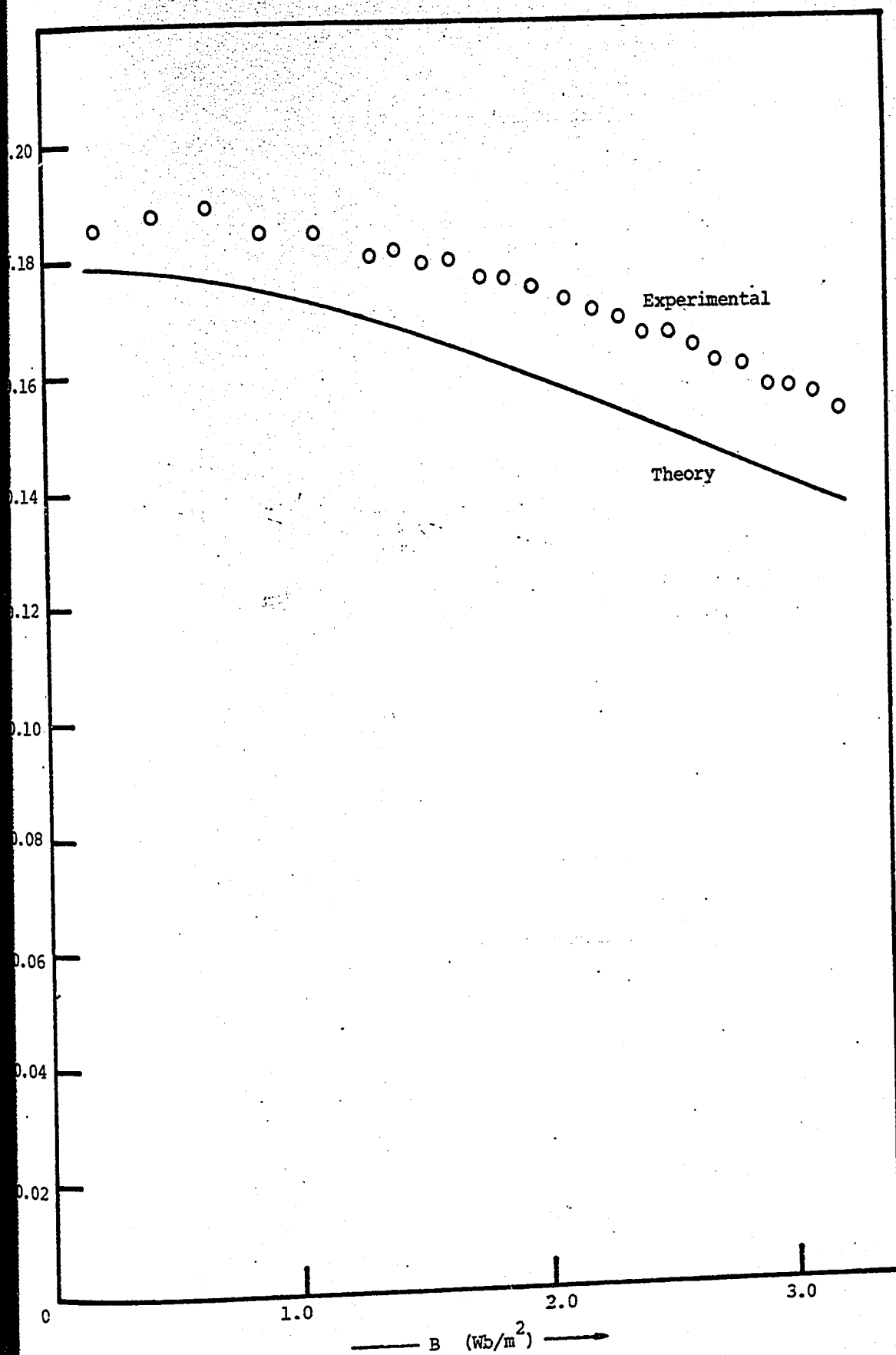


Figure 7.5. Transverse N.-E. coefficient and theory using specific relaxation times for GaSb

TABLE 7.1

Comparison of experimental and theoretical results of the longitudinal and transverse N.-E. coefficients.

	μ_1	μ_2	α_o	$\Delta\alpha(3.2 \frac{Wb}{m^2})$	$Q_{\perp}$ (Weak Field)
	$cm^2/V \text{ sec}$	$cm^2/V \text{ sec}$	$\mu V/^{\circ}K$	$\mu V/^{\circ}K$	$cm^2/^{\circ}K \text{ sec}$
Experiment	3760	491	-288	+23.8	+0.185
Theory	3776	526	-250	+23.4	+0.179
Percentage deviation with respect to experiment			13.2%	1.7%	3.2%

Résumé of theoretical scattering model

used to obtain the above results.

(ooo) band

- i) Intraband optical.
- ii) Interband optical, $D_{12} = 4.4 \times 10^8 \text{ eV/cm}$ (adjusted).
- iii) Acoustic, $E_1 = 8 \text{ eV}$.
- iv) Ionized impurity, $N_I = 2.1 \times 10^{18}/\text{cc}$.
- v) Space-charge, $N_{S^+} Q_S = 2.9 \times 10^6 \text{ m}^{-1}$ (adjusted).

<111> band

- i) Intraband optical.
- ii) Intervalley, $D_{jj'} = 7.0 \times 10^8 \text{ eV/cm}$ (adjusted).
- iii) Acoustic, $E_1 = 10 \text{ eV}$ (adjusted).
- iv) Ionized impurity, $N_I = 2.3 \times 10^{18}/\text{cc}$.

Note that the transverse N.-E. coefficient, Q_1 , in (63S2), goes from + 0.16 through a maximum of about + 0.19 and then decreases to + 0.15. The present results therefore agree well with those. It is also necessary to stress, as seen from table 7.1, that the analysis was restricted by the mobility values μ_1 and μ_2 .

Considering now the theory used to describe the 2-band case of the thermomagnetic effects, one finds that it has definite imposed limits. It is only valid under the following conditions: spherical energy surfaces, independent energy bands, isothermal conditions and relaxation time approximation.

In the case of GaSb, with the anisotropy of the L_{1c} band described by $K = m_L/m_T = 8.6$, the utilisation of the theory for spherical energy surfaces should be a good approximation. Tsidil'kovski, (62T2), mentions that in Ge, for example, with $K = 17$, the anisotropy parameters which enter into the theory of the thermomagnetic effects are quite close to unity for the single band case. It follows that in such cases, the anisotropic phenomena can be dealt with quite satisfactorily by means of the isotropic formulae. Also, in a one-band case, the longitudinal N.-E. coefficient (classical statistics and high fields) is not different whether the energy surfaces are spherical or ellipsoidal; as for the transverse N.-E. coefficient (low fields),

the theory for spherical energy surfaces predicts larger values than the theory for ellipsoidal energy surfaces. Assuming that these comments apply also to the 2-band case, the anisotropy of the L_{1c} band can probably be taken into account to a good extent through the use of the density of states and conductivity effective masses, except for $\alpha(0)$.

The condition of uncoupled bands enunciated above is not so restrictive as it might appear at first glance. Physically, we may indeed have interaction in the form of interband scattering. It is apparent that, for example, if transport in each band can be described by a relaxation time and by a steady-state carrier density, then the bands are uncoupled mathematically. A carrier scattered from band 2 to band 1 is immediately replaced by a carrier scattered into 2 by the inverse transition. This point has been made by Ehrenreich and Overhauser (56E1) who have investigated transport by the heavy- and light- mass valence bands in germanium.

It has been discussed previously, that the experimental conditions were not isothermal but adiabatic. Because there is no available experimental data on the value of the Righi-Leduc effect in GaSb, it is not possible to estimate the difference between the adiabatic and isothermal N.-E. coefficients using equations 5.4 and 5.5. One is limited to saying that since the electronic thermal conductivity is very small compared with the lattice thermal conductivity (66A1), this difference is certainly very small and probably negligible.

Since the measurements and the analysis have been made at room temperature, the relaxation time approximation could be a source of discrepancy, Einstein temperature, $h\nu/k$, being 336°K for GaSb. In the Γ_{1c} band, according to Matthiessen's rule, intraband optical phonons contribute 16% in limiting the mobility and 21% in the L_{1c} band.

The interband optical phonon scattering law is quite valid since the phonons concerned have an energy corresponding to a temperature of 270°K.

It should be noted also, that the treatment of polar modes which lead to the intraband scattering law is correct only for wave functions with s symmetry and therefore becomes less accurate for energies some distance from the band edge. The admixture of p functions which occurs, causes a decrease in the effectiveness of polar scattering. This effect has been neglected here and will lead to an overestimate of this effect for large energies. This is especially true in the case of the L_{1c} band.

Among the other scattering laws used, ionized impurity scattering is a possible source of errors in the theoretical analysis but these would be small. The ionized impurities limit the mobility of the Γ_{1c} band by 50% and by 32% in the L_{1c} band. This scattering law is valid under the Born approximation; that is, $Z \gg 1$ in equations 4.34 and 4.39. This assumes that the scattering produces a small perturbation of the electron motion. It is therefore valid if the potential energy of a particle in an external field is small compared with its kinetic

energy. The Born approximation is therefore always applicable to fast particles. Under the experimental condition of $T = 300^\circ\text{K}$, at kT , $Z = 2$ for the Γ_{1c} band. Since Z is proportional to the effective mass, Born's approximation is a better assumption in the case of the L_{1c} band.

However, despite these problems with respect to scattering, good fits can be made to the mobility curves and the theory of the thermomagnetic effects also provides a good fit to the experimental measurements without varying any of the parameters.

A theory of electron scattering in InSb-type semiconductors has been proposed by Korenblit and Sherstobitov (68K2), which takes account of the effect of a non-parabolic energy spectrum on the quantum - mechanical collision probability. The influence of an admixture of p functions in the wave function of a band electron on the probability of its scattering is taken into account. Closed formulae for the relaxation times have been obtained in the cases of ionized impurities, acoustical and optical lattice scattering. Unfortunately this work contains numerous mistakes and the problem has been redone by Zawadzki and Szymanska (71Z1). In this work, it is mentioned that neglecting the energy dependence due to screening in charge-center scattering leads to considerable overestimation of this mode in the thermomagnetic effects. This is why this effect has been taken into account in the present work. As for the other scattering

mechanisms, acoustic and optical lattice scattering, the relaxation time formulae used in the present work and those quoted in Zawadski and Szymanska (71Z1) have been compared and found to be in agreement. The non-correction for the inelasticity of collisions is the only point left which has not been discussed.

A theory of transport phenomena has also been developed by Korenblit and Sherstobitov (68K3) for semiconductors and semimetals with an isotropic spectrum of particle energies taking into account elastic and inelastic carrier scattering mechanisms. Unfortunately, it is valid only for degenerate materials. To calculate the transport coefficients in the case of inelastic collisions, it is usual to employ the variational method. However, Korenblit et al (68K3), point out that by dropping the assumption of a single relaxation time, the τ formalism can be easily generalized to describe transport phenomena in the inelastic scattering case. This has the immense advantage, over the usual variational procedure, that a full set of relaxation times allows the calculation of any transport phenomenon while the variational method requires special calculations for each effect separately. Although this work is inapplicable to the present one, it is important to mention that Korenblit et al (68K2) conclude by saying that the inelasticity of collisions affects very strongly the majority of the galvanomagnetic and thermomagnetic effects.

However, the mechanism of intraband polar optical scattering is responsible for only 16% of the total scattering in the Γ_{1c} band

and 21% in the L_{1c} band. Therefore, in this particular case, the inelasticity of the collisions affect the results only very slightly.

As is shown by the good agreement between theory and experiment, the model, used to describe the scattering in the two conduction band GaSb, is seen to give a good description of the scattering processes.

CHAPTER 8

GENERAL SUMMARY

A simple apparatus has been designed to measure, at room temperature, both the magneto-Seebeck and the transverse N.-E. effects. The problem of imperfect thermal contacts has been reduced to a minimum by using a thin piece of sapphire as the electrical insulator and thin sheets of indium in order to improve the thermal conduction. Comparing with other methods of measurements, good agreement of the electron effective mass values has been obtained on the alloy system of $\text{Ga In}_x \text{As}_{1-x}$; it can therefore be said that the experimental set-up is satisfactory.

The magneto-Seebeck coefficients of the $\text{Ga In}_x \text{As}_{1-x}$ alloys have been measured. Assuming that the conduction band of those alloys satisfies the Kane model, the electron effective mass m_o^* at the bottom of the (ooo) conduction band has been calculated as well as the scattering parameter s . The variation of m_o^* with x exhibited an almost linear behaviour with a small parabolic deviation. The scattering parameter s varied from + 0.5 to + 0.3 in going from InAs towards 60% of GaAs. This indicated that polar optical scattering was the main scattering mechanism with an increasing contribution from a mechanism having a negative scattering parameter in going from InAs towards $x = 0.6$.

The general equation for the magneto-Seebeck coefficient has been used to fit the whole curve of α vs B instead of using only $\alpha(\infty)$ and $\alpha(0)$; this verified that the empirical relation of Shalyt, used to obtain the infinite field value of α , is satisfactory.

The transverse N.-E. coefficient has then been interpreted using the general equation for this effect and it was shown that inhomogeneities affected the measurements to a large extent in this alloy system.

It has then been shown, using the general theory of the magneto-Seebeck effect, that indeed, the main scattering mechanism is polar optical scattering with a possible maximum contribution of 28% near $x = 0.6$, from either of alloy scattering or space-charge scattering.

The magneto-Seebeck and transverse N.-E. coefficients have also been measured on doped, n-type, GaSb. A theory involving two-conduction band parameters, on the assumptions of spherical energy surfaces and non-parabolic bands, has then been used in order to interpret the experimental results. A reasonable model has been suggested to describe the scattering mechanism involved in GaSb.

It has been put forward that in the Γ_{1c} band, a combination of polar optical phonons, intraband and interband, ionized impurities, acoustic phonons and space-charge and in the L_{1c} band, a combination of optical phonons, intraband and intervalley, ionized impurities and acoustic phonons succeeded in describing the complex situation of scattering in GaSb since correct mobility values were obtained. Furthermore,

when the model was used in a two-band thermomagnetic theory, the experimental results were quite well explained.

It has then been discussed that this model was quite good. The relaxation time approximation describing the polar optical scattering and the restrictions imposed on the theory of the thermomagnetic effects together with the non-inclusion of the admixture of s- and p-type wave functions in the theory of the scattering laws and the limited validity of Born's approximation at low energies, at room temperature, were shown to have little effect on the final results.

APPENDIX 3.1

DERIVATION OF Q_n^*

Q_n^* is defined in chapter 3 as:

$$Q_n^* = \frac{Q}{J_N} = \frac{Q}{J_n / -e} \quad [1]$$

The current density in the x-direction, J_{nx} can be obtained from:

$$J_{nx} = -e \int n(k) f v_x dk \quad [2]$$

where $n(k)dk$ is the number of states per unit volume with k in the element dk , v_x is the velocity in the x-direction and f is the distribution function disturbed from equilibrium by the electric field E_x .

Through the use of Boltzmann's equation, it is possible to show that:

$$J_{nx} = - \frac{2e^2 E_x}{3m_n} \int_0^\infty \xi_n \tau_n(\xi_n) \left(\frac{\partial f_0}{\partial \xi_n} \right) D_n(\xi_n) d\xi_n \quad [3]$$

where $D_n(\xi_n) d\xi_n$ is the density of states in the conduction band; it is proportional to $\xi_n^{1/2}$.

The particle current density J_{Nx} is therefore:

$$J_{Nx} = \frac{J_{nx}}{-e} = \frac{2e E_x}{3m_n} \int_0^\infty \tau_n \xi_n D_n(\xi_n) \left(\frac{\partial f_0}{\partial \xi_n} \right) d\xi_n \quad [4]$$

If the energy per particle is $(E_c + \xi_n)$, the thermal current density is:

$$\begin{aligned} Q_x &= \frac{2e E_x}{3m_n} \int_0^\infty \tau_n \xi_n (E_c + \xi_n) D_n(\xi_n) \left(\frac{\partial f_0}{\partial \xi_n} \right) d\xi_n \\ &= J_N (E_c + Q_n^*) \end{aligned} \quad [5]$$

Dividing equation [5] by equation [4]:

$$Q_n^* = \frac{Q_x}{J_{Nx}} = \frac{\int_0^\infty \tau_n (\xi_n^2 + \xi_n E_c) D_n(\xi_n) \left(\frac{\partial f_0}{\partial \xi_n} \right) d\xi_n}{\int_0^\infty \tau_n \xi_n D_n(\xi_n) \left(\frac{\partial f_0}{\partial \xi_n} \right) d\xi_n} \quad [6]$$

Defining, for the use of chapter 3 only, the mean value of any quantity, say y , over the conduction band as:

$$\langle y \rangle = \frac{\int_0^\infty y D_n(\xi_n) \left(\frac{\partial f_0}{\partial \xi_n} \right) d\xi_n}{\int_0^\infty D_n(\xi_n) \left(\frac{\partial f_0}{\partial \xi_n} \right) d\xi_n} \quad [7]$$

then,

$$Q_n^{*'} = \frac{\langle \tau_{nn}^2 \rangle}{\langle \tau_{nn} \rangle} + \frac{\langle \tau_{nn} E_c \rangle}{\langle \tau_{nn} \rangle} \quad [8]$$

and

$$Q_n^{*'} = Q_n^* + E_c \quad [9]$$

APPENDIX 4.1

CALCULATION OF $\partial n_i / \partial \zeta$ INVOLVED IN EQUATION 4.42

The electron density n_i is generally expressed as:

$$n_i = \frac{1}{\pi^2} \int_0^{\infty} f_0 k^2 \frac{dk}{dE} dE \quad [1]$$

Substituting k and dk/dE in equation [1], using the equation for a parabolic band, one obtains

$$n_{\text{parabolic}} = 4\pi \left(\frac{2m^*}{h^2} \right)^{3/2} \int_0^{\infty} f_0 E^{1/2} dE \quad [2]$$

and

$$n_{\text{parabolic}} = 4\pi \left(\frac{2m^* kT}{h^2} \right)^{3/2} F_{1/2}(\zeta) \quad [3]$$

where $F_{1/2}(\zeta)$ is the standard Fermi-Dirac integral, defined as:

$$F_n(\zeta) = \int_0^{\infty} \frac{x^n dx}{1 + e^{x-\zeta}} \quad [4]$$

or

$$(kT)^{n+1} F_n(\zeta) = \int_0^{\infty} f_0 E^n dE \quad [5]$$

If however, the energy band is non-parabolic, using equation 4.12, equation [1] can then be expressed in terms of Fermi-Dirac integrals as:

$$n_{\text{non-parabolic}} = 4\pi \left(\frac{2m_0^* kT}{h^2} \right) f(\zeta) \quad [6]$$

where

$$f(\zeta) = F_{1/2}(\zeta) + \left[\frac{5}{2} - 5\gamma \right] \beta F_{3/2}(\zeta) + \left[\frac{7}{8} - \frac{21}{2}\gamma \right] \beta^2 F_{5/2}(\zeta) - \left[\frac{1}{4} + \frac{7}{2}\gamma \right] \beta^3 F_{7/2}(\zeta)$$

$$\text{with } \gamma = m^*/m_0$$

$$\text{and } \beta = kT/E_0^*$$

The derivatives of equations [3] and [6] can be calculated using the property of the Fermi-Dirac functions:

$$\frac{\partial F_p(\zeta)}{\partial \zeta} = p F_{p-1}(\zeta) \quad [7]$$

$p > 0$

As applied to GaSb

This approach has been used in this thesis in the case of GaSb and applied to the Γ_{1c} band. The carrier concentration n_i was chosen as the total carrier concentration so as to include the effect of screening by the heavy electrons of the $\langle 111 \rangle$ band.

Therefore,

$$\frac{\partial n_i}{\partial \zeta} = \frac{\partial n_1}{\partial \zeta} + \frac{\partial n_2}{\partial \zeta} \quad [8]$$

where n_1 and n_2 are respectively the carrier concentrations in the non-parabolic (ooo) band and in the parabolic $\langle 111 \rangle$ band.

One should note that in the case of n_2 which will be described by equation [3], the multiplicity M of the $\langle 111 \rangle$ band has to be included explicitly.

Finally,

$$\frac{\partial n_1}{\partial \zeta} = 4\pi \left(\frac{2m_{01}^* kT}{h^2} \right)^{3/2} f'(\zeta) \quad [9]$$

where

$$f'(\zeta) = \frac{1}{2} F_{-1/2}(\zeta) + \frac{3}{2} \left[\frac{5}{2} - 5\gamma \right] \beta F_{1/2}(\zeta) + \frac{5}{2} \left[\frac{7}{8} - \frac{21}{2}\gamma \right] \beta^2 F_{3/2}(\zeta) - \frac{7}{2} \left[\frac{1}{4} - \frac{7}{2}\gamma \right] \beta^3 F_{5/2}(\zeta)$$

$$\text{with } \beta = m_{01}^*/m$$

and

$$\frac{\partial n_2}{\partial \zeta} = 16\pi \left(\frac{2m^* kT}{h^2} \right)^{3/2} \frac{1}{2} F_{-1/2} \left(\zeta - \frac{E_{FL}}{kT} \right) \quad [10]$$

APPENDIX 6.1

CALCULATION OF τ_0 INVOLVED IN EQUATION 4.50

The conductivity σ can be expressed as:

$$\sigma = ne\mu \quad [1]$$

$$= ne^2 \frac{\langle \tau/m^* \rangle}{\langle 1 \rangle} \quad [2]$$

$$= ne^2 \frac{\int_0^\infty \left(-\frac{\partial f_0}{\partial E} \right) \tau/m^* k^3 dE}{\int_0^\infty \left(-\frac{\partial f_0}{\partial E} \right) k^3 dE} \quad [3]$$

Using equations 4.50 and 4.5 for τ and m^* ,

$$\sigma = \left(\frac{e^2}{3\pi^2 \hbar} \right) \tau_0 \int_0^\infty \left(-\frac{\partial f_0}{\partial E} \right) k^{2s+1} \left(\frac{dE}{dk} \right)^2 dE \quad [4]$$

Solving equation [4] for τ_o ,

$$\tau_o = \frac{3\sigma \pi^2 \hbar^2}{e^2} \left[\frac{1}{\int_0^\infty \left(-\frac{\partial f_o}{\partial E} \right) k^{2s+1} \left(\frac{dE}{dk} \right)^2 dE} \right] \quad [5]$$

Equation [5] means that if the conductivity σ is known, assuming a value for s and a value for E_F , τ_o can be calculated.

S E L E C T E D R E F E R E N C E S

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