

FREE CARRIER FARADAY ROTATION IN SOME III-V
MATERIALS

by

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STATEMENT OF ORIGINALITY

The free carrier Faraday Rotation phenomenon was used to obtain the variation with alloy composition, of the effective mass of electrons at the bottom of the (000) conduction band. The results obtained from these measurements represent an original contribution. Combined with the work on magneto-thermoelectric power and infrared reflectivity the graphs for the $\text{InSb}_{1-x}\text{As}_x$ and $\text{In}_{1-x}\text{Ga}_x\text{Sb}$ alloy systems are the first consistent and reliable set of curves.

The method of analysis of the data also inherently yielded values for the variation with alloy composition, of the momentum matrix element, P^2 . These are also original results.

The combination of the Faraday effect measurements and previous magnetoresistance measurement on some single crystal GaSb specimens presented evidence for the first time that the energy separation between the (000) and $\langle 111 \rangle$ conduction band minima is function of the doping of the GaSb specimen. These measurements also yielded a value for the transverse effective mass of the $\langle 111 \rangle$ conduction band electrons which is consisted with previously reported values obtained from other theoretical and experimental analyses.

ABSTRACT

Room temperature free carrier Faraday Rotation measurements have been made on some n-type III-V materials. The data were analysed under the basic assumption that the (000) conduction band can be represented by the Kane dispersion relation. The experimental data could thus be fitted to a conduction band model of this type by adjusting the parameters E_0^* , the effective mass band gap and P^2 , the momentum matrix element. If values for Δ_0 , the spin-orbit splitting at Γ , are known, the effective mass ratio of electrons at the (000) conduction band edge, m_{00}^*/m , can be found. For the alloy specimens of the $\text{InSb}_{1-x}\text{As}_x$ and $\text{In}_{1-x}\text{Ga}_x\text{Sb}$ systems the variation with alloy composition, x , of both P^2 and m_{00}^*/m have been found.

The data from the Faraday rotation measurements on some n-type single crystal GaSb specimens were combined with previous magneto-resistance data. The analysis yielded a value for the transverse effective mass ratio of the $\langle 111 \rangle$ conduction electrons, m_{1t}/m and the scattering parameter, s . It was found that for GaSb the energy separation between the (000) and $\langle 111 \rangle$ conduction band minima, ΔE , is dependent on the degree of doping of the specimen, y , and that ΔE has a small negative temperature coefficient. Values for $\frac{d}{dy} \Delta E$ and $\frac{d}{dT} \Delta E$ are given in the thesis.

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CHAPTER 1

I N T R O D U C T I O N

i) Historical Background:

In 1845¹ Michael Faraday noticed that when plane polarised light was propagated through a slab of "heavy" glass in the presence of a longitudinal magnetic field, the plane of polarisation was rotated. Since this discovery, the Faraday effect has been observed in many gases, liquids and solids but the theory and the mechanism of this phenomenon was not well understood until the formulation of Maxwell's "Dynamical theory of the electromagnetic field" in 1864 and the discovery of the Zeeman effect in 1896. It was shortly after this that Lorentz, Drude and Voigt presented their classical dispersion theories and from these a greater understanding was achieved of the Faraday effect and other magneto-optical phenomena in terms of the motion of an electron in a magnetic field. The relation between the dispersion and the Faraday effect was first given by Becquerel² in 1897 as,

$$\theta = \frac{1}{2} \omega \omega_c \frac{dn}{d\omega}$$

where ω_c is known as the cyclotron resonance frequency, ω is the angular frequency of the radiation and n is the refractive index of the specimen. In the early twentieth century numerous measurements of the Faraday

effect were made on a number of materials³ in order to verify Becquerel's formula. These measurements however, showed the formula to be both quantitatively and qualitatively inadequate since rotations of opposite signs were observed. Since then very few magneto-optical measurements were made until the early 1950's when research on semiconducting materials began in earnest.

The discovery of the semiconducting property was made by Michael Faraday in 1833 when he found that the temperature coefficient of resistance of silver sulphide was negative. In 1874, F. Braun and A. Schuster made the first investigations on rectifying systems using mostly natural crystals such as lead sulphide and copper oxide. Since then technological interest in semiconducting materials increased but the theoretical aspect of these materials was not well understood. In 1925, Bloch⁴ presented his paper on the motion of electrons in a periodic field and this led to the concept of band structure in semiconductors. In the early 1950's a quantum mechanical interpretation of the physical phenomena in semiconductors became possible and the use of magneto-optical effects as a tool for investigating the band structure was realised.

In 1953 microwave cyclotron resonance measurements were made on Ge and Si⁵ and infra-red cyclotron resonance, which requires high pulsed field techniques for observation, was first measured on InSb⁶ in 1956. The experimental conditions however, for detecting infra-red resonances in other materials were very difficult to achieve. Mitchell⁷ in 1955 suggested that, in the dispersion term of Becquerel's formula,

there should be a contribution due to free carriers and in 1958, Smith and Moss⁸ made the first free carrier Faraday rotation measurements on InSb. These measurements showed that the rotation due to free carriers is proportional to the square of the radiation wavelength used, and this effect was shown to be independent of scattering processes and dependent only on the shapes of the energy bands. This phenomenon has become a very useful tool for investigating band structure parameters since the stringent experimental requirements of low temperatures and single crystals to reduce scattering effects ($\omega_c \tau > 1$) prohibits the observation of cyclotron resonance in many cases.

ii) Elementary Band Theory:

Since most solids are crystalline to some degree, the potential associated with the lattice has generally been regarded as being i) constant throughout the lattice, ii) periodic with the periodicity of the lattice or iii) quasi-periodic. In calculations of electronic wave functions and their corresponding energy levels, for solid state systems the ions are considered to be at rest and the potential of the lattice is that associated with the ions. The problem thus reduces to calculating the single electron wavefunction for an electron moving in a potential field caused by the ions and some average charge distribution of all other valence electrons and assuming that the wavefunction of the system is a combination of these single electron wavefunctions. In real crystals the motion of the ions can be included as a perturbation.

If a constant potential is assumed as in the Sommerfeld model, the electrons subjected to this field can be represented by plane wavefunctions of the form $\psi_k = A \exp(ikx)$ in one dimension, where k is the wavevector defining each electron. The corresponding energy values are found to be $E = \frac{\hbar^2 k^2}{2m}$. This variation of energy with wavevector is shown in fig. (1; 1(a)).

For a periodic potential in one dimension, however, solutions of the Schrödinger equation were shown by Bloch⁴ to be of the form $\psi_k = u_k(x) \exp(ikx)$ where $u_k(x)$ also has the periodicity of the lattice. Energy variations with k now have discontinuities at $k = \pm \frac{n\pi}{a}$ where a is the lattice parameter. In fig. (1; 1(b)) these discontinuities show

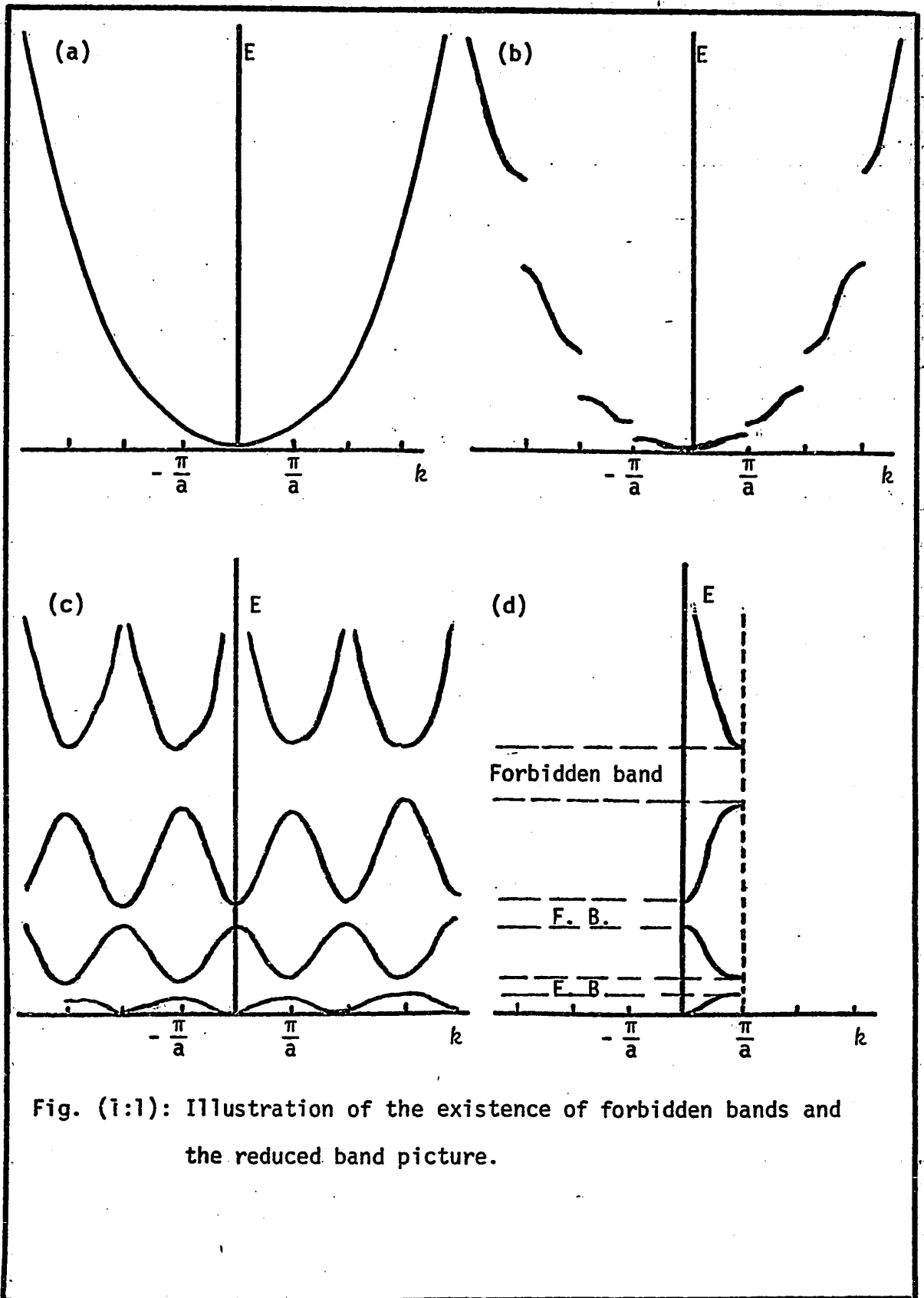


Fig. (i:1): Illustration of the existence of forbidden bands and the reduced band picture.

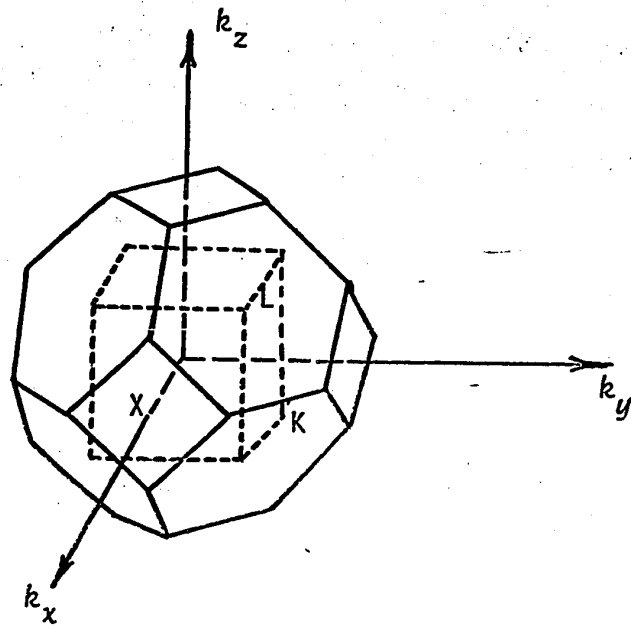
that at these critical values of k there are forbidden energy values.

Furthermore, since there is a solution of the Schrödinger equation at some k there must also be a solution at $(k \pm \frac{n\pi}{a})$ so that the E vs k curves can be fully drawn out. This extended band picture is shown in fig. (1; 1(c)). The region between $k = 0$ and $k = \frac{\pi}{a}$ is thus seen to show all the allowed energy values and hence it is only necessary to show this region to describe the complete energy system. The "reduced band" picture is shown in fig.(1; (d)).

In three dimensions it is found that for every direction in normal space discontinuities in energy exist for particular values of (k_x, k_y, k_z) . These are critical k values. If the first critical k values for all directions in normal space are plotted in k -space the result will be a surface of some shape enclosing all allowed energy states up to the first discontinuity. This surface is known as the "first Brillouin boundary" and the enclosed volume is the "first Brillouin zone". Fig. (1; 2(a)) shows the first Brillouin zone of the face centered cubic lattice. Each point in the Brillouin zone corresponds to a quantum state.

The variation of energy with wave-vector in three dimensions is generally shown in two ways. Firstly, specific directions in k -space are chosen and the "reduced band" picture is made use of, in order to show all the allowed and forbidden energy values. This type of representation is known as the "band structure diagram". For most cubic semiconductors the extrema in the energy variations lie in the directions possessing the

(a)



(b)

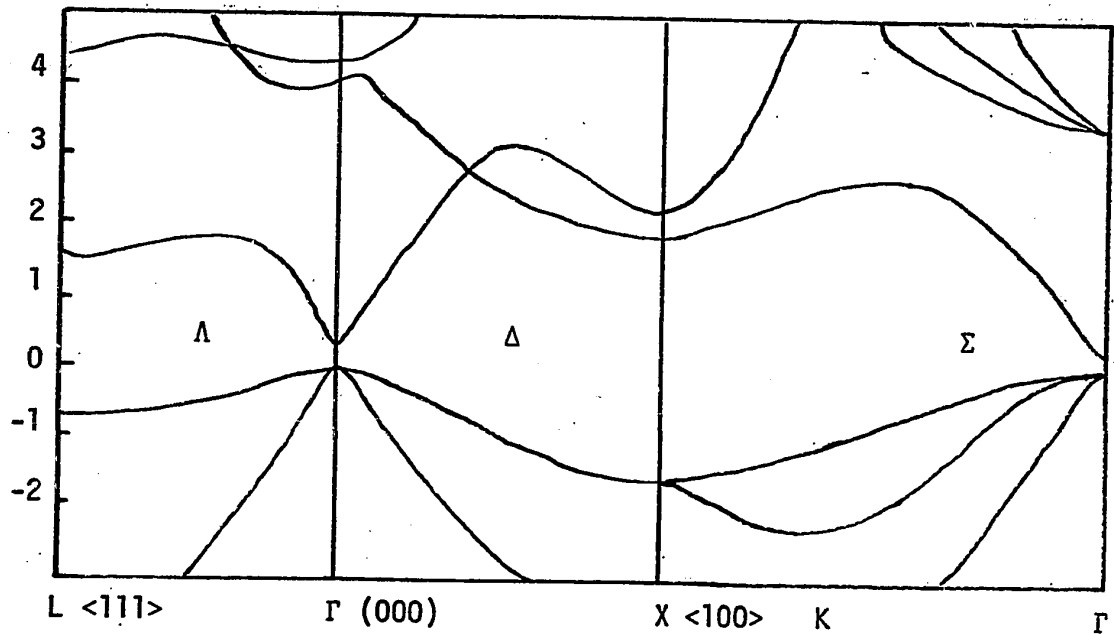


Fig. (1:2): First Brillouin zone of the f.c.c. lattice (a).

Band structure of InSb (b).

highest symmetry such as the $\langle 111 \rangle$ and $\langle 100 \rangle$ directions. Band structure diagrams are generally drawn from the (000) point in the zone to the Brillouin zone edge in these directions. In fig. (1; 2(b)) the band structure of InSb is shown together with the group theoretical notations for certain areas and points of the Brillouin zone.

The second method of showing energy variations is to plot in k -space all values of k which have the same energy values for all directions in normal space. This results in constant energy surfaces. For cubic materials in the directions of high symmetry these surfaces are seen to be either spheres centered about the center of the zone, or ellipsoids of revolution centered about the points at the zone edges.

Most research on semiconductors is aimed at deriving information about the band structure of each material. Both experimental and theoretical work is directed towards the evaluation of band parameters such as the energy separation between bands, the shapes of these bands and the number of occupied states.

iii) Element, Compound and Alloy Semiconductors:

As has been mentioned above, the first experimental measurements of band parameters were made on Germanium and Silicon⁵. These element semiconductors have diamond like crystal structures. The diamond lattice is a face centered cubic lattice and consists of two interpenetrating face-centered sub-lattices displaced from one another along a body diagonal by $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$. This kind of lattice possesses a high degree of symmetry, including an inversion center. The band structure arising from this type of lattice is shown in fig. (1; 3(a)) and has certain features due to the crystalline symmetry properties, for example the triply degenerate valence bands at the center of the Brillouin zone (Γ point) and the doubly degenerate conduction bands at the zone edge in the $\langle 100 \rangle$ direction (X point). If spin-orbit effects are taken into account one of the triply degenerate valence bands is split off a small energy below the other two. The lower band has spherical constant energy surfaces at Γ while the other two have "warped" constant energy surfaces. For Ge the nearest conduction band minima to the valence band are the four minima at the $\langle 111 \rangle$ zone edge (L-point). For Si the lowest conduction bands are the six minima in the $\langle 100 \rangle$ direction near the X-point. The constant energy surfaces at these conduction band minima are ellipsoids of revolution for both Ge and Si⁹⁻¹⁴. Ge has a higher conduction band minimum at the Γ point but this is not the case in Si¹⁵.

Since this thesis is concerned with the properties of III-V compounds and alloys, a brief review will be given of these materials only.

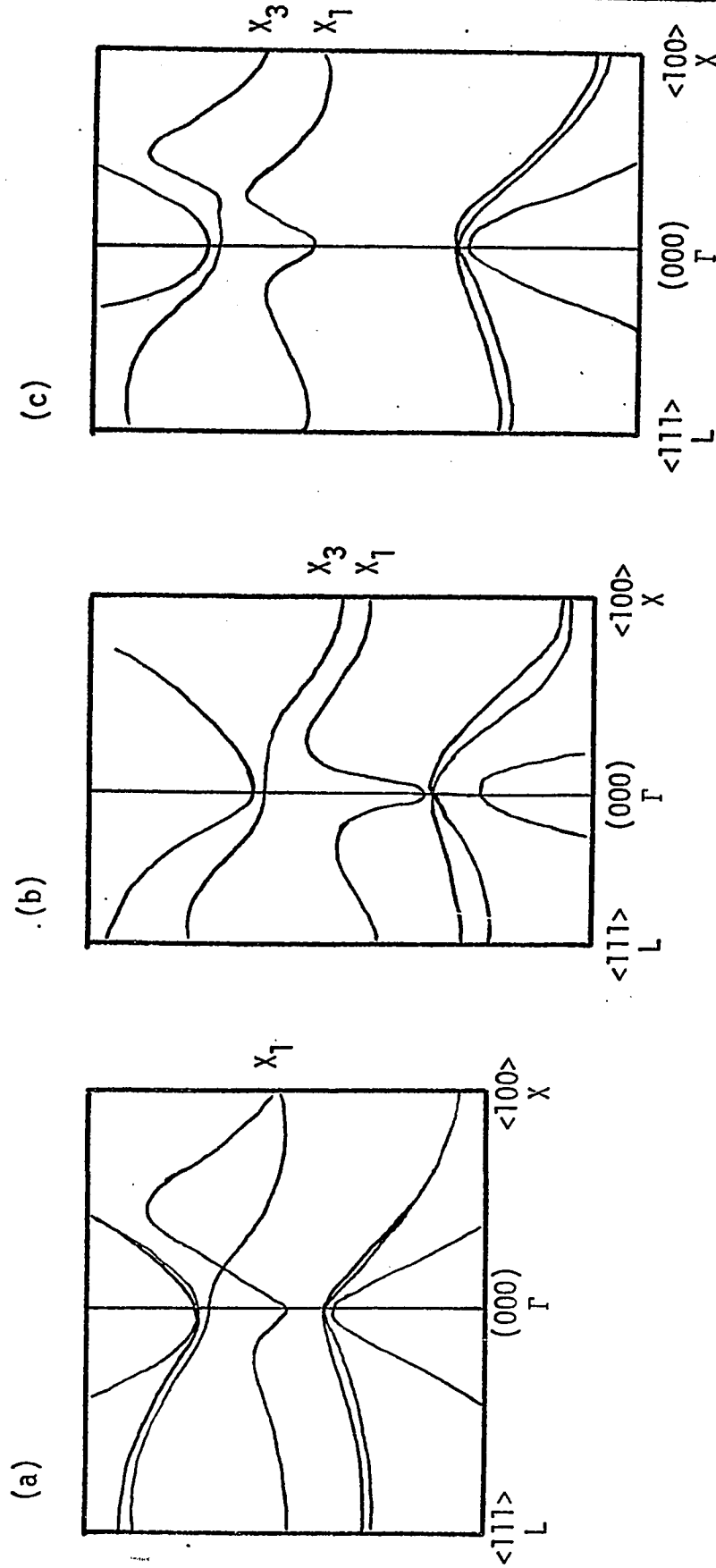


Fig. (1:3): Band structure of Ge (a). See reference 67. Band structure of InSb (b). See reference 69.
Band structure of GaP (c). See reference 73.

All the III-V compounds crystallise in the zinc blende structure. This is very similar to the diamond structure since the lattice is also face centered cubic, but here the two interpenetrating sub-lattices are formed by different atoms. Although the zinc blende structure possesses a high degree of symmetry it does not have an inversion center. Group theoretical calculations show that the lack of this symmetry element causes a lifting of the degeneracy of the $\langle 100 \rangle$ bands. The band structure diagrams of InSb and GaP are shown in figures (1; 3(b)) and (1; 3(c)).

Numerous electrical, optical and magneto-optical measurements have been made on InSb, InAs, InP, GaSb, GaAs, GaP and AlSb. A good review of this work is given by Madelung¹⁶. These investigations show that for the indium compounds, GaSb and GaAs the nearest conduction band minimum to the valence band is at the Γ point. Threshold optical transitions in these materials have been shown to be direct transitions. For GaP and AlSb however the threshold transitions are indirect and are from the valence band to a $\langle 100 \rangle$ conduction band minimum. The two materials chosen for fig. (1; 3(b)) and fig. (1; 3(c)) demonstrate this difference. Table (1A) gives a summary of the band structure parameters obtained from numerous electrical, magnetic, optical and magneto-optical experiments on III-V compounds. Furthermore, results of cyclotron resonance experiments on single crystals show that for those III-V compounds in which the threshold optical transitions are direct the constant energy surfaces for the (000) conduction band minimum are spherical and the constant energy

Parameter	InSb	InAs	GaSb	GaAs	GaP
lowest conduction band	(000)	(000)	(000)	(000)	<100>
next lowest conduction band	<111>	<111>	<111>	<100>	(000)
energy gap E_0 (eV)	0.18	0.36	0.73	1.38	2.78
Spin-orbit splitting, Δ_0 (eV)	0.82	0.38	0.82	0.35	0.10
Effective mass m_{00}^*/m	0.013	0.025	0.045	0.068	0.135

T A B L E 1A

surfaces for the secondary conduction bands are ellipsoids of revolution.

It has been postulated that the valence band maxima for the III-V compounds do not lie at the zone center but are located some distance in the $\langle 111 \rangle$ direction. Some recent results¹⁰⁷ show this to be the case in InSb but evidence to support this in other III-V materials is still forthcoming¹⁷.

The technological applications of these III-V compounds in devices has motivated an extensive search for new materials and therefore a number of laboratories have begun research programs on semiconducting alloys. As a result of this it was found that two III-V compounds could be combined to form solid solution in which only one zinc blende phase is present. This work is being actively carried on in this laboratory. A review of the preparation procedures and degree of success achieved in many III-V compounds is given by Coderre¹⁸.

The fact that the III-V semiconductor alloys are disordered can be more easily explained if the pseudo-binary system InSb-GaSb is chosen as an example. Here as small amounts of GaSb are added to InSb some of the indium atoms are substitutionally replaced by gallium atoms. This is a completely random process and is responsible for the disorder in III-V alloys. It has been found that for this system a complete range of solid solution can be obtained in which only one zinc blende phase is present at any given composition.

The calculation of the band structure of an alloy is extremely complicated and attempts to date have met with only limited success. Various workers¹⁹⁻²⁴ have used qualitative means in their treatment

of ideal one-dimensional alloys in order to find the general principles governing the energy level distribution. These studies could not give numerical results and are hence not well suited for the study of three-dimensional alloys.

The potential acting on an electron moving through a disordered alloy can be divided in two parts i) a periodic part and ii) an aperiodic part. In the "virtual crystal model", which was first introduced by Nordheim²⁵, the periodic part is the average alloy potential which is taken over all the possible configurations of atoms at any specific alloy composition, and the aperiodic part is then the deviation of the alloy potential from this average. Nordheim used this concept on one-dimensional alloys and found that the virtual crystal model predicted a linear variation of physical constants with composition from one component to the other if the aperiodic part of the potential could be treated as being zero.

The linear variation of the lattice parameter was also predicted by another law, called Vegard's law, and a number of X-ray measurements²⁶⁻²⁹ of the variation of lattice parameter with composition in III-V alloys give results which are not inconsistent with this although positive and negative deviations from Vegard's law have been found.

The concept of the "virtual crystal model" was extended by Muto³⁰ who treated the non-periodic part of the potential as a perturbation and found that to first order the alloying effect did not change the energy levels.

Numerous other measurements have been made on semiconducting alloys in order to investigate the variation of band parameters with alloy

composition. These will be mentioned later on as the results have been used for the calculations in this thesis. It was seen that the variation with alloy composition of certain parameters such as the fundamental gap, deviates from linearity in a concave manner. Parmenter³¹⁻³³, who used the "virtual crystal model" for calculations on one-dimensional semiconductors, pointed out that any deviation from linearity predicted by this model should be due to second order perturbation and is proportional to the mean square deviation of the random perturbing potential from the average potential. These higher order effects were thus found to follow a $x(1-x)$ variation where x is the mole fraction of one component of the alloy. Parmenter further found that the effect of second and higher orders of perturbation was to "smear" the allowed energy band edges into the forbidden zone, but only to a finite extent. Hence it is still possible to assign a band structure to alloy semiconductors as long as the disordering effect produced by the formation of the alloy is small enough to be considered as a perturbation.

These conclusions were first applied by Cardona³⁴ on the experimentally measured energy gaps of the alloys of the silver and cuprous halides. Cardona found that the measured deviations from linearity for this parameter fitted reasonably well on a curve of the form $Cx(1-x)$ where C is a constant.

Thompson and Woolley³⁵ applied the results of the virtual crystal model to the observed energy gaps of some III-V alloys. They showed that the fundamental gap varied with composition according to the relation

$$E_0 = \{A + B'x\} + \{Cx(1 - x)\}$$

where the first term is due to the average potential in the virtual crystal and the second term is due to the random perturbing potential. The experimental results hence showed very good agreement with a curve of the form

$$E_0 = A + Bx + Cx^2$$

where here A is the fundamental gap of one compound and $D = A + B + C$ is the fundamental gap of the other compound.

The amount of deviation from linearity was found to be dependent on the alloy system chosen and an empirical rule was found which stated that C varies inversely as the square root of the mean fundamental gap of the two compounds. i.e.

$$C = a/\{(A + D)/2\}^{\frac{1}{2}}$$

iv) Effective Mass:

The concept of effective masses has been discussed in numerous standard texts³⁶⁻³⁸. It is useful, however, to point out the differences in the various effective masses and to indicate under which conditions each type of effective mass may be derived, so as to know which of these is to be used in the analysis of the data from different measurements.

In one dimension, when an external electric field E is applied to a system of electrons moving in a crystalline potential the acceleration of these electrons can be found by representing the electrons as de Broglie waves of velocity $v = \frac{1}{\hbar} \frac{dE}{dk}$ and energy $E = \hbar\omega$. The acceleration is thus given by

$$a = \frac{1}{\hbar} \frac{d^2E}{dk^2} \frac{dk}{dt} = \frac{1}{\hbar^2} \frac{d^2E}{dk^2} \frac{d(\hbar k)}{dt} \dots\dots\dots[1:1]$$

When the electric field acts on the electron the rate at which the electron gains energy is given by

$$\frac{dE}{dt} = eEv = \frac{1}{\hbar} F \frac{dE}{dk}$$

where F is the force on the electron and can thus be written as

$F = \frac{d(\hbar k)}{dt}$. The term $\hbar k$ is called the crystal momentum. In [1:1] it can be seen that $(\frac{1}{\hbar^2} \frac{d^2E}{dk^2})^{-1}$ must have the units of mass. This mass, since

it is related to the curvature of the E vs k curves, is known as the "band curvature effective mass". This type of effective mass cannot be measured directly since it requires knowledge of the force on the electron and the acceleration of the electron. However, once the band structure is known this mass can be found.

When the applied force is due to a magnetic field, B , the electrons move in orbits. The force on the electrons is thus given by $\frac{d}{dt}(\hbar k) = ev_{\perp} B$, where $v_{\perp}$ is the velocity of the electrons in a plane perpendicular to the magnetic field and can be written as $v_{\perp} = \frac{1}{\hbar} \frac{dE}{dk_{\perp}}$. This is balanced by the centrifugal force $m^* v_{\perp}^2 / r = m^* \omega_c v_{\perp}$ where r is the radius of the orbit and ω_c is the cyclotron resonance frequency given by $\omega_c = \frac{eB}{m^*}$. Hence the period of each orbit is given by

$$\int dt = \frac{2\pi}{\omega_c} = \frac{2\pi m^*}{eB} = \frac{\hbar}{eB} \oint \frac{dk}{v_{\perp}}$$

$$m^* = \frac{\hbar^2}{2\pi} \oint \frac{dk_{\perp} dk}{dE}$$

or $m^* = \frac{\hbar^2}{2\pi} \frac{dA(k)}{dE}$ where $A(k)$ is the area in k -space bounded by the electronic orbit. If the energy surfaces are spherical it can be seen that $\frac{1}{m^*} = \frac{1}{\hbar^2} \frac{1}{k} \frac{dE}{dk}$. This is the usual expression for the "cyclotron effective mass". Experiments, such as all measurement of magneto-optical effects, will thus yield values for the cyclotron effective mass. Measurements of the cyclotron effective mass will thus yield values for the slopes of the E vs k curves. As will be seen in Chapter 2, however, these values are

sometimes difficult to interpret at room temperature since in many cases the magneto-optical phenomena are caused by electrons occupying a range of energy states and in these cases the distribution of electronic states must be taken into account. At low temperature or in degenerate specimen the energy of the electrons is more clearly defined and here an integration procedure on a number of experimental results can be used in order to find the band shape. Other measurements, such as infrared reflectivity which is a method of finding the magnetic susceptibility of a material, will also yield cyclotron effective masses.

In three dimensions the effective masses are tensor quantities and their values depend on the shapes of the constant energy surfaces in k -space. There are six components for each type of effective mass since these tensors are symmetric. For certain types of symmetry a number of these components can be reduced to zero if a suitable choice of axes is made. For instance, if the energy surfaces are spherical and the reference origin is at the centre of the sphere the effective mass is isotropic and all diagonal components are equal. If the constant energy surfaces are ellipsoids of revolution and the axes of reference lie along the axes of these ellipsoids of revolution then only two different diagonal components appear. These are usually referred to as two equal transverse components and one longitudinal component. For both types of energy surfaces all the off-diagonal components reduce to zero if the above axes are chosen.

For all the III-V materials considered in this thesis and the alloys

of these materials the energy surfaces about the centre of the Brillouin zone are spherical and those about the zone edges, $\langle 111 \rangle$ or $\langle 100 \rangle$, are ellipsoids of revolution. Hence for the (000) conduction band the one dimensional effective masses formerly described are suitable as long as the spherical constant energy surface approach is valid. This is generally the case when doping levels are not excessive. For the $\langle 111 \rangle$ or $\langle 100 \rangle$ band, however, new definitions must be found. Considering one set of ellipsoidal energy surfaces, previous workers have derived expressions for the Faraday and reflectivity effective masses³⁹⁻⁴². If the energy bands are parabolic the effective mass is independent of the wave vector k and depends only on the shape of the constant energy surface. The expressions arrived at are thus averages over the transverse effective mass, m_{it}^* , and the longitudinal effective mass, m_{il}^* . The following are the results given in the literature.

$$\left(\frac{1}{m_{iF}^*}\right)^2 = \frac{1}{3m_{it}^*} \left(\frac{1}{m_{it}^*} + \frac{2}{m_{il}^*}\right) \dots \dots \dots [1:2]$$

and
$$\frac{1}{m_{iR}^*} = \frac{1}{3} \left(\frac{1}{m_{il}^*} + \frac{2}{m_{it}^*}\right) \dots \dots \dots [1:3]$$

where $i = 0, 1$ or 2 signifies the (000), $\langle 111 \rangle$ and $\langle 100 \rangle$ conduction bands respectively, m_{iF}^* is the Faraday rotation effective mass and m_{iR}^* is the reflectivity effective mass. If $K_i = m_{il}^*/m_{it}^*$ is a measure of the shape of the energy surfaces then [1:2] and [1:3] reduce to

$$m_{iF}^* = m_{i\ell} \{3K_i/(K_i + 2)\}^{\frac{3}{2}} \dots \dots \dots [1:4]$$

and $m_{iR}^* = m_{i\ell} \{3K_i/(1 + 2K_i)\} \dots \dots \dots [1:5]$

For the (000) band $m_{o\ell} = m_{o\ell}$ and at the bottom of the band, using the above expressions, $m_{oF}^* = m_{oR}^* = m_{oo}^*$, which is the bottom of the band effective mass.

The expressions for the effective masses given above are derived by considering the action of an electric or a magnetic field on electrons with specified energy E. In reality the applied fields act on a large number of electrons which in general have a wide range of energy values. An equation can be derived which relates the number of electrons to the Fermi energy. The parameter by which the number of electrons and the Fermi energy can be related has the dimensions of mass and is an average effective mass known as the "density of states" effective mass.

As has been mentioned in section (ii) of this chapter, every point in the first Brillouin zone represents a quantum state. The number of electrons having an energy between E and E + dE is thus given by

$$dN(E) = 2d\Omega_k \dots \dots \dots [1:6]$$

where $d\Omega_k$ is a volume element in k-space and the factor 2 arises from the double degeneracy of each state when electronic spin is considered.

If the constant energy surfaces around the centre of the first

in k -space is parabolic, i.e. $E = \frac{\hbar^2 k^2}{2m_{on}^*}$, equation [1:6] can be written as

$$dN(E) = 8\pi k^2 dk$$

or
$$dN(E) = (4\pi/\hbar^3)(2m_{on}^*)^{\frac{3}{2}} E^{\frac{1}{2}} dE$$

and on integrating over energy from 0 to the Fermi energy E_{Fi} , the concentration of electrons per unit volume, n_i , is related to the Fermi energy by

$$n_i = (8\pi/3\hbar^3)(2m_{on}^*)^{\frac{3}{2}} E_{Fi}^{\frac{3}{2}} \dots \dots \dots [1:7]$$

This is the well known "density of states" equation and, if the E vs k relation is parabolic, equation [1:7] defines the "density of states" effective mass. For the case of spherical energy surfaces and non-parabolic bands the density of states mass is given in the literature⁴³ as being an average of the cyclotron effective mass, m_{oc}^* , and the simple parabolic "density of states" effective mass given above. i.e. $m_{od}^* = (m_{on}^* m_{oc}^*)^{\frac{1}{2}}$.

When the energy surfaces are ellipsoids of revolution and the energy bands are parabolic as is the case for the $\langle 111 \rangle$ and $\langle 100 \rangle$ bands, the density of states mass, m_{id}^* , is given by⁴⁴

$$m_{id}^* = (m_{il} m_{it}^2)^{\frac{1}{3}} \dots \dots \dots [1:8]$$

The density of states equations for these more complicated forms of band structure will be shown in Chapter 2, however, it can be seen here

that the effective masses to be used in these equations are the density of states masses m_{od}^* and m_{id}^* . These equations since they concern the total number of electrons can be used in the analysis of Hall effect data.

The following nomenclature will be used in this thesis for the various types of effective masses.

Band curvature	$m_{ob}^* = \frac{\hbar^2}{(d^2E/dk^2)}$
Cyclotron	$m_{oc}^* = \frac{\hbar^2 k}{(dE/dk)}$
Simple density of states	$m_{on}^* = \frac{\hbar^2 k^2}{2E}$
Density of states	$m_{od}^* = (m_{on}^* m_{oc}^{*2})^{1/3}$
Bottom of the band	m_{oo}^*

(These refer to the (000) band since, for the III-V compounds used in this thesis, these constant energy surfaces are spherical. These bands however, are non-parabolic).

Transverse	$m_{it}; \quad \begin{array}{l} i = 1 \text{ } \langle 111 \rangle \text{ band} \\ i = 2 \text{ } \langle 100 \rangle \text{ band} \end{array}$
Longitudinal	$m_{il}; \quad (i = 1, 2)$
Density of states	$m_{id}^* = (m_{il} m_{it}^2)^{1/3}; (i = 1, 2)$

These bands can be treated as being parabolic, and the energy surfaces are ellipsoids of revolution.

The effective masses measured by free carrier Faraday rotation (m_{iF}^*) and infrared reflectivity (m_{iR}^*) will both reduce to the cyclotron effective mass, m_{oc}^* , evaluated at the Fermi level, for highly degenerate (000) bands. The $\langle 111 \rangle$ and $\langle 100 \rangle$ band definitions for these effective masses are seen in [1:2] and [1:3].

From the above it is clear that a knowledge of effective mass values gives important information about the conduction band structure and the shapes of the constant energy surfaces. For non-parabolic bands the effective masses change from the bottom of the band value to higher values as the conduction states are filled. In this thesis, therefore, the variation of the bottom of the (000) conduction band effective mass, m_{oo}^* , will be found for alloy material and the variation of m_{oo}^* with alloy composition will be shown. In this way each measurement is normalised to the bottom of the (000) band.

v) Alloy Research:

The advantages gained from the study of alloy semiconductors are of both a technological and academic nature. The main physical parameters contributing to the usefulness of semiconductors are the fundamental energy gap and the effective mass values of electrons and holes in the various bands. The effectiveness of a semiconductor as a light emitter, optical detector, optical filter, microwave generator or a laser, is primarily determined by these parameters.

Since semiconductor alloys show a smooth variation of these parameters with composition the ability to manufacture these materials and to investigate the band structure parameters is of great importance.

Certain physical quantities are difficult to measure in materials such as GaSb where the (000) and $\langle 111 \rangle$ conduction band minima are close together^{45,46}. Alloying GaSb with another material where these two bands are more separated in energy, such as InSb, enables one to study the band structure from the InSb rich end and by working towards the GaSb rich end a knowledgeable estimate of band parameters of GaSb can be found.

There are a number of measurements which can be made on these alloys in order to study the variation of band parameters with composition. The semiconductor group at this university is now actively involved in various magnetic, electrical, optical and thermal measurements. In the case of the alloys presented in this thesis at least one other measurement besides Faraday rotation has been made. In this way a consistent set of values has

be found for the variation of one band parameter, namely the bottom of the (000) conduction band effective mass, m_{00}^* . Free carrier Faraday rotation is purely a dispersive effect and does not depend on the relaxation times or scattering mechanism. This rotation is however, in principle always accompanied by a degree of ellipticity which is caused by the differential attenuation of the two circular components making up the incident plane polarised radiation. This is dependent on the relaxation time, τ , and measurement of both effects, the rotation and ellipticity, can yield values for τ^{108} . This has not been attempted here but some information on the predominant scattering mechanism has been obtained by combining the Faraday rotation results with the results from magneto-thermoelectric power measurements^{4,7}

In order to facilitate the reading of this thesis a brief outline of the scope and objectives of this work will now be given.

The investigation of the free carrier Faraday effect in III-V materials has been carried out in order to obtain values for the variation with alloy composition for the bottom of the (000) band effective mass. The theoretical expressions necessary for the analysis of the data is given and, in some cases, derived in Chapter 2. The necessary ancillary measurements to be made become clear once these expressions are known.

In Chapter 3 the experimentation is described for each measurement made and the data obtained is listed in Chapter 4. The method of analysis of data is dependent on the specimen measured. The introduction to Chapter 5 illustrates which methods of analysis are to be used. The data and analysis results are given in categories of compounds and alloys. A summary of these and some concluding remarks are then given in Chapter 6.

CHAPTER 2

T H E O R Y

i) Introduction:

As has been mentioned before, the free carrier Faraday effect has become increasingly more useful in the study of band structure parameters. The simplest way to explain this phenomenon is to consider the plane polarized wave in the medium to be split up into two oppositely polarised circular components. On the application of a magnetic field along the direction of propagation of the radiation, each of the two circularly polarised waves "sees" a different refractive index and hence their velocities in the specimen are different. If the anticlockwise rotation (observer looking towards the radiation) is taken to be the positive wave and the clockwise component the negative wave it can be shown that the rotation θ is related to the wavelength λ of the radiation by

$$\theta = \frac{\pi t}{\lambda}(\eta_- - \eta_+)$$

where t is the specimen thickness and $\eta_{\pm}$ are the refractive indices of the specimen for the negative and positive components of the radiation respectively.

At the wavelengths generally used for observing free carrier Faraday rotation in semiconductors η_- and η_+ are only slightly different and

$(\eta_-^2 - \eta_+^2) \approx 2\eta(\eta_- - \eta_+)$ where η is the refractive index of the specimen at wavelength λ in zero magnetic field. The rotation is thus given by

$$\theta = \frac{\pi t}{2\eta\lambda}(\eta_-^2 - \eta_+^2) \dots \dots \dots [2:1]$$

There are two methods which are generally used to express the free carrier rotation in terms of the band structure and these will be described in more detail in the next sections. Both these methods make use of equation [2:1] but in the first method a semi-classical approach yields the rotation in terms of the cyclotron effective mass which, as has been seen in Chapter 1, can be related to the band structure. In the second method a more detailed treatment starting from the Boltzmann transport equation gives an expression for the free carrier rotation in terms of the variation of energy in k -space and the distribution of electronic states. Here, as will be seen, some model for the conduction band must be chosen.

ii) Semi-classical Theory:

From the Drude-Zener theory and the solution of the equation of motion of the deflection of electrons by two circularly polarised waves and a magnetic field parallel to the direction of propagation of the radiation, the complex refractive index of the medium is given by

$$(\eta_{\pm} - i\kappa_{\pm})^2 = \epsilon_r + \left(\frac{n_i e^2}{m_{ic}^* \omega \epsilon_0} \right) / \left(-\omega \pm \frac{Be}{m_{ic}^*} \pm \frac{i}{\tau} \right) \dots \dots \dots [2:2]$$

in the m.k.s. system of units. Here ϵ_r is the specific dielectric constant of the material in the absence of free carriers, n_i is the number of free carriers, ω is the angular frequency of the radiation, ϵ_0 is the permittivity of free space (8.8542×10^{-12} farads/m), B is the magnetic field, τ is the relaxation time which is part of the damping term in the equation of motion and m_{ic}^* is the effective mass of the electrons. Since free carrier Faraday rotation is a measure of the differential dispersion due to cyclotron resonance absorption, the effective mass used here is the cyclotron effective mass.

The differential dispersion can thus be found from the real part of equation [2:2] which is given by

$$\eta_{\pm}^2 - \kappa_{\pm}^2 = \epsilon_r - \frac{n_i e^2}{m_{ic}^* \omega \epsilon_0} \left[\frac{\omega \pm \omega_c}{(\omega \pm \omega_c)^2 + 1/\tau^2} \right] \dots \dots \dots [2:3]$$

where $\omega_c = \frac{Be}{m_{ic}^*}$.

Assuming that the absorption is small so that $\eta_{\pm}^2 \gg \kappa_{\pm}^2$ and under the conditions that $\omega^2 \gg \omega_c^2$ and $\omega\tau \gg 1$ it can be shown that

$$(\eta_-^2 - \eta_+^2) = \frac{n_i e^2}{m_{ic}^* \epsilon_0} \left(\frac{2eB}{m_{ic}^* \omega^3} \right)$$

or

$$(\eta_-^2 - \eta_+^2) = \frac{n_i e^3 B \lambda^3}{4\pi^3 c^3 \epsilon_0 m_{ic}^{*2}}$$

and hence using equation [2:1]

$$\theta = \frac{n_i e^3 t B \lambda^2}{8\pi^2 c^3 \epsilon_0 \eta m_{ic}^{*2}}$$

in radians and this can be written as

$$\theta = 1.509 \times 10^{-11} \frac{B t n_i \lambda^2}{\eta (m_{ic}^*/m)^2} \dots\dots\dots [2:4]$$

in the m.k.s. system and here θ is in degrees. Hence the free carrier Faraday effect shows a linear dependence on the square of the wavelength with the straight line extrapolating through the origin. The rotation is seen to be independent of the relaxation time and therefore no knowledge of the electron scattering mechanism is required and furthermore, since the rotation depends on the inverse square of the effective mass this type of measurement is a potentially accurate way of finding the effective mass.

The investigation of the variation of the cyclotron effective mass with the doping level of the specimen can thus be carried out using the free carrier Faraday effect. This variation can be related to the shape of the conduction band since the cyclotron effective mass is defined by the term $(\frac{1}{k} \frac{dE}{dk})$. Stephen and Lidiard⁴⁰ have shown that for spherical energy surfaces and high degeneracy i.e. for a semiconductor in which the Fermi level E_{Fi} is more than $4kT$ above the conduction band minimum⁴⁸, the effective mass must be interpreted as

$$\frac{1}{m_{ic}^*} = \frac{1}{\hbar^2} \frac{1}{k_{Fi}} \left. \frac{dE}{dk} \right|_{Fi} \dots\dots\dots [2:5]$$

where the subscript Fi means that the effective mass is evaluated at the Fermi level. Under the same conditions of spherical energy surfaces and high degeneracy the value of the Fermi radius k_{Fi} can be found from the Hall effect since here the relation between the carrier concentration and the Fermi radius is given by⁴⁹

$$k_{Fi}^3 = 3\pi^2 n_i \dots\dots\dots [2:6]$$

Measurements of free carrier Faraday effect and Hall effect on a number of degenerate specimens of the same compound will thus yield values of the Fermi radius and the slope of the energy band at the Fermi radius. An integration of this curve will then give the band shape. This type of procedure has been carried out on InSb by Smith et al⁴⁹.

In the case of non-degenerate specimens and spherical constant energy surfaces equations [2:5] and [2:6] cannot be used since here many states are contributing to the rotation. The cyclotron effective mass measured by free carrier Faraday rotation measurements on these specimens is therefore a mean effective mass averaged over the occupied states. This case will be dealt with in the following section.

iii) Statistical Theory:

The expression for the Faraday rotation in terms of the distribution of states has been given by previous workers^{40,50} and a complete derivation can be found in reference 106. For the sake of completeness and in order to indicate the approximations made in the derivation it is deemed useful to present this theory in its entirety.

There are three basic steps to the solution of this problem.

- a) The rotation is first expressed in terms of the conductivity of a semiconductor in the presence of an alternating electric field and a static magnetic field.
- b) Using the Boltzmann transport equation the conductivity is related to the band structure and the distribution functions.
- c) The results of (a) and (b) are then combined and the Faraday rotation is expressed in terms of the band structure and the distribution of states.

a) The Conductivity: In the m.k.s. system, Maxwell's field equations for a conducting medium are

$$\vec{\nabla} \times \vec{E} = -\mu_r \mu_0 \frac{\partial \vec{H}}{\partial t}$$

$$\vec{\nabla} \times \vec{H} = \vec{J} + \epsilon_r \epsilon_0 \frac{\partial \vec{E}}{\partial t}$$

$$\vec{\nabla} \cdot \vec{H} = 0$$

$$\vec{\nabla} \cdot \vec{E} = 0$$

Here μ_0 is the permeability of free space ($4\pi \times 10^{-7}$ henries/m), ϵ_0 is the permittivity of free space (8.8542×10^{-12} farads/m), μ_r is the specific permeability and ϵ_r is the dielectric constant or specific permittivity. By manipulating the above equations $\vec{H}$ can be eliminated and an expression involving the electric field $\vec{E}$ is

$$\nabla^2 \vec{E} - \mu_r \mu_0 \frac{\partial \vec{J}}{\partial t} - \mu_r \mu_0 \epsilon_r \epsilon_0 \frac{\partial^2 \vec{E}}{\partial t^2} = 0 \dots \dots \dots [2:7]$$

In the presence of static magnetic fields, $\vec{H}$, the components of the current density $\vec{J}$ may be written as

$$J_i = \Sigma_{ij} E_j + \Sigma_{ijk} H_k E_j$$

where Σ_{ij} and Σ_{ijk} are generalised tensors as introduced by Abeles and Meiboom³⁹.

For cubic crystals, symmetry requires that

$$\Sigma_{ij} = \sigma \delta_{ij} \text{ and } \Sigma_{ijk} = \sigma' \epsilon_{ijk}$$

where δ_{ij} is the Kronecker delta and ϵ_{ijk} is the substitution tensor. Hence

$$J_i = \sigma \delta_{ij} E_j + \sigma' \epsilon_{ijk} E_j H_k \dots \dots \dots [2:8]$$

where σ and σ' are complex quantities given by

$$\sigma = \sigma_r + i\sigma_i \text{ and } \sigma' = \sigma'_r + i\sigma'_i \dots\dots\dots[2:9]$$

The components of $\vec{J}$ are thus given by

$$J_i = (\sigma_r + i\sigma_i)\delta_{ij}E_j + (\sigma'_r + i\sigma'_i)\epsilon_{ijk}E_jH_k \dots\dots\dots[2:10]$$

Using [2:8] in [2:7] the field equation can be seen to be

$$\nabla^2 \vec{E} - \mu_r \mu_0 \left[\sigma \frac{\partial \vec{E}}{\partial t} + \sigma' \frac{\partial}{\partial t} (\vec{E} \times \vec{H}) \right] - \mu_r \mu_0 \epsilon_r \epsilon_0 \frac{\partial^2 \vec{E}}{\partial t^2} = 0$$

and since $\vec{H}$ is static

$$\nabla^2 \vec{E} - \mu_r \mu_0 \left[\sigma \frac{\partial \vec{E}}{\partial t} + \sigma' \frac{\partial \vec{E}}{\partial t} \times \vec{H} \right] - \mu_r \mu_0 \epsilon_r \epsilon_0 \frac{\partial^2 \vec{E}}{\partial t^2} = 0 \dots\dots\dots[2:11]$$

If the applied magnetic field is in the z direction and the experimental set-up is for the Faraday effect, i.e. plane polarised radiation is propagated parallel to the applied magnetic field then $E_z = 0$ and E_x and E_y are finite and are given by

$$E_{\pm} = E_x \pm iE_y$$

where

$$E_{\pm} = E_{0\pm} \exp \frac{i\omega}{c}(N_{\pm}r + ct) \dots\dots\dots[2:12]$$

are the two circularly polarised components of the plane polarised radiation. The signs are defined as in section (i) of this chapter, and $N_{\pm}$ is the complex refractive index of the medium.

The x and y components of equation [2:10] are

$$\frac{\partial^2 E_x}{\partial x^2} - \mu_r \mu_0 \sigma \frac{\partial E_x}{\partial t} - \mu_r \mu_0 \sigma' \frac{\partial E_y}{\partial t} H_z - \mu_r \mu_0 \epsilon_r \epsilon_0 \frac{\partial^2 E_x}{\partial t^2} = 0$$

and

$$\frac{\partial^2 E_y}{\partial y^2} - \mu_r \mu_0 \sigma \frac{\partial E_y}{\partial t} + \mu_r \mu_0 \sigma' \frac{\partial E_x}{\partial t} H_z - \mu_r \mu_0 \epsilon_r \epsilon_0 \frac{\partial^2 E_y}{\partial t^2} = 0$$

Multiplying the second equation by $\pm i$ and adding gives

$$\frac{\partial^2 E_{\pm}}{\partial r^2} - \mu_r \mu_0 \sigma \frac{\partial E_{\pm}}{\partial t} \pm i \mu_r \mu_0 \sigma' \frac{\partial E_{\pm}}{\partial t} H_z - \mu_r \mu_0 \epsilon_r \epsilon_0 \frac{\partial^2 E_{\pm}}{\partial t^2} = 0$$

Using [2:9] and [2:12] in the above equation and solving for $N_{\pm}^2$ one gets

$$N_{\pm}^2 = \mu_r \mu_0 c^2 \left[\epsilon_r \epsilon_0 + \frac{\sigma_i}{\omega} \mp \frac{\sigma'_r H_z}{\omega} - i \left(\frac{\sigma_r}{\omega} \pm \frac{\sigma'_i H_z}{\omega} \right) \right] \dots \dots \dots [2:13]$$

The complex refractive index is given by

$$N_{\pm} = \eta_{\pm} - i \kappa_{\pm} \dots \dots \dots [2:14]$$

where as in the previous sections $\eta_{\pm}$ is the refractive index of the medium for the two circularly polarised components and $\kappa_{\pm}$ is known as the

extinction coefficient. Hence $\eta_{\pm}$ is the real part of $N_{\pm}$ and $\kappa_{\pm}$ is the imaginary part of $N_{\pm}$. Making use of the mathematical identities that for a complex number A

$$(\operatorname{Re} A)^2 = \frac{1}{2} \left[\operatorname{Re}(A^2) + \sqrt{(\operatorname{Re}(A^2))^2 + (\operatorname{Im}(A^2))^2} \right]$$

and
$$(\operatorname{Im} A)^2 = \frac{1}{2} \left[-\operatorname{Re}(A^2) + \sqrt{(\operatorname{Im}(A^2))^2 + (-\operatorname{Re}(A^2))^2} \right]$$

in [2:13] the expressions for $\eta_{\pm}$ and $\kappa_{\pm}$ are given by

$$\eta_{\pm}^2 = \frac{c^2 \mu_r \mu_0}{2} \left[\left(\epsilon_r \epsilon_0 + \frac{\sigma_i}{\omega} \mp \frac{H_z \sigma'_r}{\omega} \right) + \sqrt{\left(\epsilon_r \epsilon_0 + \frac{\sigma_i}{\omega} \mp \frac{H_z \sigma'_r}{\omega} \right)^2 + \left(\frac{\sigma_r}{\omega} \pm \frac{H_z \sigma'_i}{\omega} \right)^2} \right]$$

and

$$\kappa_{\pm}^2 = \frac{c^2 \mu_r \mu_0}{2} \left[\left(-\epsilon_r \epsilon_0 - \frac{\sigma_i}{\omega} \pm \frac{H_z \sigma'_r}{\omega} \right) + \sqrt{\left(\epsilon_r \epsilon_0 + \frac{\sigma_i}{\omega} \mp \frac{H_z \sigma'_r}{\omega} \right)^2 + \left(\frac{\sigma_r}{\omega} \pm \frac{H_z \sigma'_i}{\omega} \right)^2} \right]$$

.....[2:15]

On substituting the expression for $\eta_{\pm}^2$ in [2:1], the Faraday angle θ is given by

$$\theta = \frac{\pi t}{2\eta\lambda} \left[\frac{c^2 \mu_r \mu_0}{2} \left\{ \left(\epsilon_r \epsilon_0 + \frac{\sigma_i}{\omega} + \frac{H_z \sigma'_r}{\omega} \right) - \left(\epsilon_r \epsilon_0 + \frac{\sigma_i}{\omega} - \frac{H_z \sigma'_r}{\omega} \right) + \right. \right. \\ \left. \sqrt{\left(\epsilon_r \epsilon_0 + \frac{\sigma_i}{\omega} + \frac{H_z \sigma'_r}{\omega} \right)^2 + \left(\frac{\sigma_r}{\omega} - \frac{H_z \sigma'_i}{\omega} \right)^2} - \right. \\ \left. \left. \sqrt{\left(\epsilon_r \epsilon_0 + \frac{\sigma_i}{\omega} - \frac{H_z \sigma'_r}{\omega} \right)^2 + \left(\frac{\sigma_r}{\omega} + \frac{H_z \sigma'_i}{\omega} \right)^2} \right\} \right]$$

$$\theta = \pi t \frac{c^2 \mu_r \mu_0}{4 \eta \lambda} \left[2 H_z \frac{\sigma_r'}{\omega} + \sqrt{\left(\epsilon_r \epsilon_0 + \frac{\sigma_i}{\omega} \right)^2 + 2 \left(H_z \frac{\sigma_i}{\omega} \frac{\sigma_r'}{\omega} + H_z \epsilon_r \epsilon_0 \frac{\sigma_r'}{\omega} - H_z \frac{\sigma_r}{\omega} \frac{\sigma_i'}{\omega} \right) + \left(H_z \frac{\sigma_r'}{\omega} \right)^2 + \left(\frac{\sigma_r}{\omega} \right)^2 + \left(H_z \frac{\sigma_i'}{\omega} \right)^2} \right. \\ \left. - \sqrt{\left(\epsilon_r \epsilon_0 + \frac{\sigma_i}{\omega} \right)^2 + 2 \left(H_z \frac{\sigma_r}{\omega} \frac{\sigma_i'}{\omega} - H_z \frac{\sigma_i}{\omega} \frac{\sigma_r'}{\omega} - H_z \epsilon_r \epsilon_0 \frac{\sigma_r'}{\omega} \right) + \left(H_z \frac{\sigma_r'}{\omega} \right)^2 + \left(\frac{\sigma_r}{\omega} \right)^2 + \left(H_z \frac{\sigma_i'}{\omega} \right)^2} \right]$$

$$\theta = \frac{t \omega c^2 \mu_r \mu_0}{8 \eta c} \left[2 H_z \frac{\sigma_r'}{\omega} + \sqrt{\left\{ \left(\epsilon_r \epsilon_0 + \frac{\sigma_i}{\omega} \right)^2 + \left(\frac{\sigma_r}{\omega} \right)^2 \right\} + 2 H_z \frac{\sigma_r'}{\omega} \left\{ \left(\frac{\sigma_i}{\omega} + \epsilon_r \epsilon_0 \right) - \frac{\sigma_i'}{\sigma_r'} \left(\frac{\sigma_r}{\omega} \right) \right\} + \left(H_z \frac{\sigma_r'}{\omega} \right)^2 + \left(H_z \frac{\sigma_i'}{\omega} \right)^2} \right. \\ \left. - \sqrt{\left\{ \left(\epsilon_r \epsilon_0 + \frac{\sigma_i}{\omega} \right)^2 + \left(\frac{\sigma_r}{\omega} \right)^2 \right\} + 2 H_z \frac{\sigma_r'}{\omega} \left\{ \left(\frac{\sigma_r}{\omega} \right) \frac{\sigma_i'}{\sigma_r'} - \left(\frac{\sigma_i}{\omega} + \epsilon_r \epsilon_0 \right) \right\} + \left(H_z \frac{\sigma_r'}{\omega} \right)^2 + \left(H_z \frac{\sigma_i'}{\omega} \right)^2} \right] \\ \dots\dots\dots[2:16]$$

In the absence of fields $\eta_{\pm}^2 = \eta^2$; $\kappa_{\pm}^2 = \kappa^2$ and $H_z = 0$ and hence from

[2:15]

$$2\eta^2 = c^2 \mu_r \mu_0 \left[\left(\epsilon_r \epsilon_0 + \frac{\sigma_i}{\omega} \right) + \sqrt{\left(\epsilon_r \epsilon_0 + \frac{\sigma_i}{\omega} \right)^2 + \left(\frac{\sigma_r}{\omega} \right)^2} \right] \dots\dots\dots[2:17a]$$

$$2\kappa^2 = c^2 \mu_r \mu_0 \left[-\left(\epsilon_r \epsilon_0 + \frac{\sigma_i}{\omega} \right) + \sqrt{\left(\epsilon_r \epsilon_0 + \frac{\sigma_i}{\omega} \right)^2 + \left(\frac{\sigma_r}{\omega} \right)^2} \right] \dots\dots\dots[2:17b]$$

$$2\eta\kappa = c^2 \mu_r \mu_0 \left(\frac{\sigma_r}{\omega} \right) \dots\dots\dots[2:17c]$$

$$\eta^2 - \kappa^2 = c^2 \mu_r \mu_0 \left(\epsilon_r \epsilon_0 + \frac{\sigma_i}{\omega} \right) \dots\dots\dots[2:17d]$$

$$(\eta^2 + \kappa^2)^2 = c^4 \mu_r^2 \mu_0^2 \left\{ \left(\epsilon_r \epsilon_0 + \frac{\sigma_i}{\omega} \right)^2 + \left(\frac{\sigma_r}{\omega} \right)^2 \right\} \dots\dots\dots[2:17e]$$

Now using equations [2:17] in [2:16] and the low field approximation (i.e. terms in H_z^2 are neglected) one gets

$$\begin{aligned} \theta &= \frac{t\omega c^2 \mu_r \mu_0}{8\eta c} \left[2H_z \frac{\sigma_r'}{\omega} + \sqrt{\left(\frac{\eta^2 + \kappa^2}{c^2 \mu_r \mu_0}\right)^2 + 2H_z \frac{\sigma_r'}{\omega} \left\{ -\frac{2\eta\kappa}{c^2 \mu_r \mu_0} \left(\frac{\sigma_i'}{\sigma_r'}\right) + \left(\frac{\eta^2 - \kappa^2}{c^2 \mu_r \mu_0}\right) \right\}} \right. \\ &\quad \left. - \sqrt{\left(\frac{\eta^2 + \kappa^2}{c^2 \mu_r \mu_0}\right)^2 + 2H_z \frac{\sigma_r'}{\omega} \left\{ \frac{2\eta\kappa}{c^2 \mu_r \mu_0} \left(\frac{\sigma_i'}{\sigma_r'}\right) + \left(\frac{\eta^2 - \kappa^2}{c^2 \mu_r \mu_0}\right) \right\}} \right] \\ &= \frac{t\omega c^2 \mu_r \mu_0}{8\eta c} \left[2H_z \frac{\sigma_r'}{\omega} + \sqrt{\left(\frac{\eta^2 + \kappa^2}{c^2 \mu_r \mu_0}\right)^2 + 2H_z \frac{\sigma_r'}{\omega} \left\{ \frac{-2\eta\kappa\sigma_i' + \sigma_r'(\eta^2 - \kappa^2)}{\sigma_r' c^2 \mu_r \mu_0} \right\}} \right. \\ &\quad \left. - \sqrt{\left(\frac{\eta^2 + \kappa^2}{c^2 \mu_r \mu_0}\right)^2 + 2H_z \frac{\sigma_r'}{\omega} \left\{ \frac{2\eta\kappa\sigma_i' + \sigma_r'(\eta^2 - \kappa^2)}{\sigma_r' c^2 \mu_r \mu_0} \right\}} \right] \\ &= \frac{t\omega c^2 \mu_r \mu_0}{8\eta c} \left[2H_z \frac{\sigma_r'}{\omega} + \left(\frac{\eta^2 + \kappa^2}{c^2 \mu_r \mu_0}\right) \sqrt{1 + 2H_z \frac{\sigma_r'}{\omega} \left\{ \frac{\sigma_r'(\eta^2 - \kappa^2) - 2\eta\kappa\sigma_i'}{\sigma_r' c^2 \mu_r \mu_0} \right\} \frac{c^4 \mu_r^2 \mu_0^2}{(\eta^2 + \kappa^2)^2}} \right. \\ &\quad \left. - \left(\frac{\eta^2 + \kappa^2}{c^2 \mu_r \mu_0}\right) \sqrt{1 + 2H_z \frac{\sigma_r'}{\omega} \left\{ \frac{2\eta\kappa\sigma_i' - \sigma_r'(\eta^2 - \kappa^2)}{\sigma_r' c^2 \mu_r \mu_0} \right\} \frac{c^4 \mu_r^2 \mu_0^2}{(\eta^2 + \kappa^2)^2}} \right] \end{aligned}$$

The factor under the square root is now expanded and terms in H_z^2 are again neglected. Hence

$$\begin{aligned} \theta &= \frac{t\omega c^2 \mu_r \mu_0}{8\eta c} \left[2H_z \frac{\sigma_r'}{\omega} + \left(\frac{\eta^2 + \kappa^2}{c^2 \mu_r \mu_0}\right) \left\{ 1 + \frac{H_z}{\omega} \frac{c^2 \mu_r \mu_0}{(\eta^2 + \kappa^2)^2} \left(\frac{\sigma_r'(\eta^2 - \kappa^2) - 2\eta\kappa\sigma_i'}{1} \right) \right. \right. \\ &\quad \left. \left. - 1 - \frac{H_z}{\omega} \frac{c^2 \mu_r \mu_0}{(\eta^2 + \kappa^2)^2} \left(\frac{2\eta\kappa\sigma_i' - \sigma_r'(\eta^2 - \kappa^2)}{1} \right) \right\} \right] \end{aligned}$$

$$\begin{aligned}
 \theta &= \frac{t\omega c^2 \mu_r \mu_0}{8\eta c} \left[2H_z \frac{\sigma_r'}{\omega} + \frac{H_z}{\omega} \frac{1}{(\eta^2 + \kappa^2)} (-2\eta\kappa\sigma_i' + \sigma_r'(\eta^2 - \kappa^2) + \sigma_r'(\eta^2 - \kappa^2) - 2\eta\kappa\sigma_i') \right] \\
 &= \frac{t\omega c^2 \mu_r \mu_0}{8\eta c} \left[2H_z \frac{\sigma_r'}{\omega} + \frac{2H_z}{\omega} \left(\frac{\sigma_r'\eta^2 - \sigma_r'\kappa^2 - 2\eta\kappa\sigma_i'}{\eta^2 + \kappa^2} \right) \right] \\
 &= \frac{t\omega c \mu_r \mu_0 H_z}{4\omega} \left[\frac{1}{\eta} \left(\frac{\sigma_r'\eta^2 + \sigma_r'\kappa^2 + \sigma_r'\eta^2 - \sigma_r'\kappa^2 - 2\eta\kappa\sigma_i'}{\eta^2 + \kappa^2} \right) \right] \\
 &= \frac{t\omega c \mu_r \mu_0 H_z}{4} \left\{ \frac{2\sigma_r'\eta - 2\sigma_i'\kappa}{\eta^2 + \kappa^2} \right\}
 \end{aligned}$$

and therefore

$$\theta = \frac{t\omega c \mu_r \mu_0 H_z}{2} \left(\frac{\sigma_r'\eta - \sigma_i'\kappa}{\eta^2 + \kappa^2} \right) \dots\dots\dots[2:18]$$

The conditions under which the Faraday effect is observed requires that $\eta^2 \gg \kappa^2$ and hence

$$\theta = \frac{t\omega c \mu_r \mu_0 H_z}{2\eta} \sigma_r' \dots\dots\dots[2:19]$$

and this is the expression which will be used.

b) Boltzmann Transport equation:

The Boltzmann transport equation for the distribution function $f(k)$ in the presence of external fields is

$$\left[\frac{\partial f(k)}{\partial t} \right]_{diff} - \left[\frac{\partial f(k)}{\partial t} \right]_{coll} = \frac{\partial f(k)}{\partial t}$$

where

$$\left[\frac{\partial f(k)}{\partial t} \right]_{diff} = \left[\frac{\partial f(k)}{\partial k} \frac{dk}{dt} \right]_{fields} + \left[\frac{\partial f(k)}{\partial r} \frac{dr}{dt} \right]_{thermal}$$

is the term due to the applied fields and the spatial dependence brought about by temperature gradients. For an isothermal metal the steady state Boltzmann equation is

$$\left[\frac{\partial f(k)}{\partial k} \frac{dk}{dt} \right]_{fields} - \left[\frac{\partial f(k)}{\partial t} \right]_{coll} = 0 \dots\dots\dots[2:20]$$

When the deviation from equilibrium is small, it is customary to assume that in the absence of external forces the rate of change of the distribution function is proportional to the deviation. The collision term in the transport equation may then be written as

$$\left[\frac{\partial f(k)}{\partial t} \right]_{\text{collisions}} = - \frac{f - f_0}{\tau} \dots\dots\dots [2:21]$$

It must be pointed out however that equation [2:21] assumes that a relaxation time can be defined. This is not strictly true. In fact the problem of defining the collision term in Boltzmann's equation is formidable and hence the above assumption is at most a practical one.

In [2:21] f_0 is the Fermi equilibrium distribution function and is given by $f_0 = \left[1 + \exp\left(\frac{E - E_{Fi}}{kT}\right) \right]^{-1}$

In the presence of electromagnetic radiation and a magnetic field the force on an electron is

$$\vec{F} = -e \left\{ \vec{E} + \vec{v} \times \vec{B} \right\} = \hbar \frac{d\vec{k}}{dt}$$

Equation [2:20] becomes

$$- \frac{e}{\hbar} \left\{ \vec{E} + \vec{v} \times \vec{B} \right\} \cdot \vec{\nabla}_k f(k) + \frac{f(k) - f_0}{\tau} = 0 \dots\dots\dots [2:22]$$

In the presence of external forces the distribution function is generally written as

$$f = f_0 - \Phi \frac{\partial f_0}{\partial E} \dots\dots\dots [2:23]$$

Using [2:22] and [2:23] a general equation ϕ is given (Wilson⁵¹) as

$$\frac{\phi}{\tau} + \frac{e}{\hbar} \vec{E} \cdot \vec{\nabla}_k E + \frac{e}{\hbar^2} \vec{B} \cdot \vec{\nabla}_k E \times \vec{\nabla}_k \phi = 0$$

and a solution for ϕ has been obtained by Jones and Zener⁵² who used an iterative procedure and found that

$$\phi = \left[-\frac{e}{\hbar} \left\{ \tau \vec{E} \cdot \vec{\nabla}_k E - \frac{e}{\hbar^2} \tau \vec{B} \cdot \vec{\nabla}_k E \times \vec{\nabla}_k (\tau \vec{E} \cdot \vec{\nabla}_k E) \dots + \right. \right. \\ \left. \left. \text{higher order terms in } \vec{B} \text{ which are neglected} \right\} \right] \dots \dots \dots [2:24]$$

The current density is given by

$$d\vec{J} = -e\vec{v}dn = -\frac{ef(k)\vec{v}}{4\pi^3} dk_x dk_y dk_z$$

or

$$\vec{J} = -\frac{e}{4\pi^3} \int_0^\infty \vec{v} f(k) d^3k$$

Using equation [2:23] the current density equation becomes

$$\vec{J} = -\frac{e}{4\pi^3} \int_0^\infty \frac{1}{\hbar} \vec{\nabla}_k E (f_0 - \phi \frac{\partial f_0}{\partial E}) d^3k \\ = -\frac{e}{4\pi^3 \hbar} \left[\int_0^\infty \vec{\nabla}_k E f_0 d^3k + \int_0^\infty \vec{\nabla}_k E \phi \frac{\partial f_0}{\partial E} d^3k \right]$$

The first integral contributes very little and may be neglected.

Therefore

$$\vec{J} = - \frac{e}{4\pi^3\hbar} \int_0^\infty \vec{\nabla}_k E \cdot \Phi \frac{\partial f_0}{\partial E} d^3k$$

and using [2:24]

$$\begin{aligned} \vec{J} &= - \frac{e}{4\pi^3\hbar} \int_0^\infty \frac{\partial f_0}{\partial E} \vec{\nabla}_k E \left(- \frac{e}{\hbar} \tau \vec{E} \cdot \vec{\nabla}_k E \right) d^3k \\ &\quad + \int_0^\infty \frac{\partial f_0}{\partial E} \vec{\nabla}_k E \left[\frac{e^2}{\hbar^3} \tau \vec{B} \cdot \vec{\nabla}_k E \times \vec{\nabla}_k (\tau \vec{E} \cdot \vec{\nabla}_k E) \right] d^3k \\ &= \frac{e^2}{4\pi\hbar^2} \int_0^\infty \tau \frac{\partial f_0}{\partial E} \vec{\nabla}_k E \cdot \vec{E} \cdot \vec{\nabla}_k E d^3k \\ &\quad - \frac{e^3}{4\pi^3\hbar^4} \int_0^\infty \tau^2 \frac{\partial f_0}{\partial E} \vec{\nabla}_k E \cdot \left[\vec{B} \cdot \vec{\nabla}_k E \times \vec{\nabla}_k (\vec{E} \cdot \vec{\nabla}_k E) \right] d^3k \end{aligned}$$

In order to include the effect of an alternating $\vec{E}$, τ is replaced by⁴⁰ $(\tau^{-1} + i\omega)^{-1}$ and τ^2 is replaced by $(\tau^{-1} + i\omega)^{-2}$ which in the limit that $\omega\tau \gg 1$ reduce to $(1/\omega^2\tau) - (i/\omega)$ and $(-1/\omega^2) - (2i/\omega^3\tau)$ respectively. The current density can thus be written as

$$\vec{J} = \frac{e^2}{4\pi\hbar^2\omega^2} \int_0^\infty \frac{1}{\tau} \frac{\partial f_0}{\partial E} \vec{\nabla}_k E \cdot \vec{E} \cdot \vec{\nabla}_k E d^3k$$

$$\begin{aligned}
 & - \frac{e^2 i}{4\pi\hbar^2\omega} \int_0^\infty \frac{\partial f_0}{\partial E} \vec{\nabla}_k E \cdot \vec{E} \cdot \vec{\nabla}_k E d^3k \\
 & + \frac{e^3}{4\pi^3\hbar^4\omega^2} \int_0^\infty \frac{\partial f_0}{\partial E} \vec{\nabla}_k E \cdot \vec{B} \cdot \vec{\nabla}_k E \times \vec{\nabla}_k (\vec{E} \cdot \vec{\nabla}_k E) d^3k \\
 & + \frac{2e^3 i}{4\pi^3\hbar^4\omega^3} \int_0^\infty \frac{1}{\tau} \frac{\partial f_0}{\partial E} \vec{\nabla}_k E \cdot \vec{B} \cdot \vec{\nabla}_k E \times \vec{\nabla}_k (\vec{E} \cdot \vec{\nabla}_k E) d^3k \dots\dots\dots [2:25]
 \end{aligned}$$

Since the problem here has reduced to finding σ'_r which will later be introduced into equation [2:19] equations [2:10] and [2:25] are now compared. It can be seen that σ'_r is the coefficient of the real part of the term involving both the electric and magnetic fields to first order. On working out the components of $\vec{J}$ it can thus be shown that

$$\sigma'_r = \frac{e^3 \mu_r \mu_0}{4\pi^3 \hbar^4 \omega^2} \int_0^\infty \frac{\partial f_0}{\partial E} \cdot \frac{\partial E}{\partial k_x} \left[\frac{\partial E}{\partial k_y} \frac{\partial^2 E}{\partial k_x \partial k_y} - \frac{\partial E}{\partial k_x} \frac{\partial^2 E}{\partial k_x \partial k_y^2} \right] d^3k \dots\dots\dots [2:26]$$

c) Inserting [2:26] in [2:19] and writing $c^2 = 1/\mu_0 \epsilon_0$, $\mu_r \mu_0 H_z = B$ and $\omega^2 = 4\pi^2 c^2 / \lambda^2$ the general expression for the Faraday rotation in a cubic crystal is

$$\theta = \frac{45e^3 t B \lambda^2}{8\pi^6 \hbar^4 c^3 \epsilon_0 \eta} \int_0^\infty \frac{\partial f_0}{\partial E} \cdot \frac{\partial E}{\partial k_x} \left[\frac{\partial E}{\partial k_y} \cdot \frac{\partial^2 E}{\partial k_x \partial k_y} - \frac{\partial E}{\partial k_x} \cdot \frac{\partial^2 E}{\partial k_y^2} \right] d^3k \dots\dots\dots [2:27]$$

in the m.k.s. system and here θ is in degrees.

In order to compare [2:27] with [2:4] so that an expression for the Faraday effective mass may be found use is made of the relation for the concentration

$$n_i = \frac{2}{(2\pi)^3} \int_0^\infty f_0 d^3k \dots\dots\dots [2:28]$$

and combining [2:27] and [2:28]

$$\theta = \frac{45e^3 t B n_i \lambda^2}{2\pi^3 \hbar^4 c^3 \epsilon_0 n} \frac{I_1}{I_2}$$

where
$$I_1 = \int_0^\infty \frac{\partial f_0}{\partial E} \frac{\partial E}{\partial k_x} \left[\frac{\partial E}{\partial k_y} \frac{\partial^2 E}{\partial k_x \partial k_y} - \frac{\partial E}{\partial k_x} \frac{\partial^2 E}{\partial k_y^2} \right] d^3k$$

and
$$I_2 = \int_0^\infty f_0 d^3k$$

An expression for the Faraday effective mass is

$$(m_{iF}^*/m) = (4a^2 I_2 / I_1)^{1/2} \dots\dots\dots [2:29]$$

Equation [2:29] thus gives an average cyclotron mass which can be

measured experimentally by finding I_1 from the slope of the θ vs λ^2 lines and I_2 from a Hall effect measurement.

In order to relate I_1 and I_2 to the band structure it is necessary to adopt some model for the conduction band. In the next section the model which is used in these calculations is discussed.

Another feature to point out is that from equation [2:27] it can be seen that the rotation is again shown to be independent of the relaxation time and remains purely a dispersive effect.

iv) The Kane Theory:

The theoretical determination of band structure is generally an extremely complicated problem. The necessity of finding the band structure of materials, such as the III-V compounds, has led to a number of different approaches to this problem. In all these, however, the first step is to study the crystal structure of the material and then, using group theory, the symmetry of the crystal structure can give a qualitative idea about the energy bands and the degeneracy of these bands. Spin effects can also be included at this point and these indicate which degeneracies are lifted. These calculations cannot give quantitative information about the shapes of the energy bands. With the above symmetry calculations as a foundation, however, more quantitative theories can be developed and the energy band schema can be found, either in the vicinity of a symmetry point or for a complete zone in certain important symmetry directions. One approximation which always must be made is that the problem can be reduced to a "one-electron" case where the presence of all other electrons is somehow taken into consideration.

A theory such as this was worked out by Kane^{53,54} for Ge and InSb. Kane used the $\vec{k} \cdot \vec{p}$ perturbation approach^{13,55,56}, and he pointed out⁵⁴ that since the $\vec{k} \cdot \vec{p}$ representation involves a large number of parameters this method is not as practical for a complete zone analysis as is the simpler pseudopotential method developed by Phillips⁵⁷. The $\vec{k} \cdot \vec{p}$

representation, however, is considered to be more accurate and easier to analyse if only a small portion of the zone, in the vicinity of a symmetry point, is considered.

Since this thesis is concerned with band parameters at the conduction band minimum the $\vec{k} \cdot \vec{p}$ representation is suitable and hence the Kane model for the conduction band will be used. The development of Kane's theory will now be outlined.

The Schrödinger equation for an electron moving in a periodic potential $V(\vec{r})$ and including spin-orbit coupling is

$$\left[\frac{\vec{p}^2}{2m} + V(\vec{r}) + \frac{\hbar}{4m^2c^2} (\vec{\nabla}V(\vec{r}) \times \vec{p}) \cdot \vec{\sigma} \right] \psi_k = E_k \psi_k \dots\dots\dots [2:30]$$

where $\vec{p}$ is the momentum operator and $\vec{\sigma}$ is the spin operator.

Using a Bloch function of the form $\psi_k = u_k(\vec{r})\exp(i\vec{k} \cdot \vec{r})$ in equation [2:30] and operating on this function with the momentum operator an equation for the lattice periodic function is

$$(H_0 + H_1 + H_2 + H_3) u_k = E_k' u_k \dots\dots\dots [2:31]$$

where $H_0 = \frac{\vec{p}^2}{2m} + V(\vec{r})$ is the Hamiltonian of the unperturbed problem

$H_1 = \frac{\hbar}{m} \vec{k} \cdot \vec{p}$ is the spin independent perturbation for small k

and
$$\left\{ \begin{array}{l} H_3 = \frac{\hbar}{4m^2c^2} (\vec{\nabla}V(\vec{r}) \times \vec{p}) \cdot \vec{\sigma} \\ H_4 = \frac{\hbar^2}{4m^2c^2} (\vec{\nabla}V(\vec{r}) \times \vec{k}) \cdot \vec{\sigma} \end{array} \right\} \text{ are spin dependent perturbations}$$

and
$$H'_k = E_k - \frac{\hbar^2 k^2}{2m}$$

In order to expand the wavefunctions of the perturbed problem in terms of the wavefunctions of the unperturbed problem Kane chooses as zero-order basis functions, two s-functions of opposite sign S_+ and S_- and six p-functions $X_{\pm}$, $Y_{\pm}$ and $Z_{\pm}$. He thus restricts the calculation to three valence and one conduction band and ignores the effects of higher and lower bands. In order that most of the matrix elements in the resultant 8x8 determinant vanish, the basis functions are derived using the symmetry properties of the crystal structure. The only parameters which remain are the separation between the valence bands and the split off spin-orbit valence band, Δ_0 , the separation between the valence bands and the conduction band, E_0 , and a momentum matrix element P^2 .

The solution of the secular determinant then results in the equation.

$$\left\{ (E + E_0 - ak^2) \right\} \left\{ (E - ak^2) (E + E_0 - ak^2) (E + E_0 + \Delta_0 - ak^2) - ak^2 P^2 (E + E_0 + \frac{2}{3} \Delta_0 - ak^2) \right\} = 0 \dots\dots\dots [2:32]$$

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

There are four solutions to this equation and at $k = 0$ $E_1 = -E_0$, $E_2 = 0$, $E_3 = -E_0$ and $E_4 = -(E_0 + \Delta_0)$. It can thus be seen that the energy E is measured from the conduction band minimum which is given by solution E_2 . E_1 and E_3 are the degenerate valence bands and E_4 is the spin-orbit split-off band.

It must be pointed out that equation [2:32] was derived without any consideration of the vibration of the lattice. The parameter E_0 , which is the fundamental gap, is thus the optically measured gap for intrinsic material only at absolute zero. At higher temperatures however this parameter is not the fundamental gap. Ehrenreich⁵⁸ pointed out that at higher temperatures this parameter is an effective energy gap called the "effective mass band gap", which would be the separation between the valence band maximum and conduction band minimum at $k = 0$ if only lattice dilatation effects are considered. Since dilatation of the lattice would change the separation between these bands as well as the shapes of these bands and interaction with the phonon field effects only the separation, Ehrenreich suggested that the Kane theory would still be applicable at higher temperatures if E_0 is replaced by E_0^* , the effective mass band gap. Neglecting the first root of [2:32] the secular equation becomes

$$(E - ak^2)(E + E_0^* - ak^2)(E + E_0^* + \Delta_0 - ak^2) - ak^2P^2(E + E_0^* + \frac{2}{3}\Delta_0 - ak^2) = 0$$

.....[2:33]

Use of equation [2:33] in the form given is not tractable and various workers have made different approximations which reduce [2:33] to more practical forms. Furthermore, since the factor P^2 is not found directly from any experiments it would be useful to replace the parameter by one which can be measured more directly, such as an effective mass. Using the definition of cyclotron effective mass given in section (iv) of chapter 1, it can be seen from [2:33] that

$$\begin{aligned}
 & \left(\frac{dE}{dk} - 2ak \right) (E + E_0^* - ak^2) (E + E_0^* + \Delta_0 - ak^2) \\
 & + (E - ak^2) \left(\frac{dE}{dk} - 2ak \right) (E + E_0^* + \Delta_0 - ak^2) \\
 & + (E - ak^2) (E + E_0^* - ak^2) \left(\frac{dE}{dk} - 2ak \right) \\
 & - 2akP^2 (E + E_0^* + \frac{2}{3} \Delta_0 - ak^2) \\
 & - ak^2P^2 \left(\frac{dE}{dk} - 2ak \right) = 0
 \end{aligned}$$

or $\left(\frac{1}{\hbar^2} \frac{1}{k} \frac{dE}{dk} - \frac{2a}{\hbar^2} \right) \left[(E + E_0^* - ak^2) (E + E_0^* + \Delta_0 - ak^2) \right.$

$$\left. + (E - ak^2) (E + E_0^* - \Delta_0 - ak^2) + (E - ak^2) (E + E_0^* - ak^2) - ak^2P^2 \right]$$

$$= \frac{2aP^2}{\hbar^2} (E + E_0^* + \frac{2}{3} \Delta_0 - ak^2)$$

At $k = 0$, $E = 0$ and the cyclotron effective mass reduces to the bottom of the band effective mass, m_{00}^* . Thus

$$\left(\frac{1}{m_{00}^*} - \frac{2a}{\hbar^2}\right) E_0^*(E_0^* + \Delta_0) = \frac{2aP^2}{3\hbar^2} (3E_0^* + 2\Delta_0)$$

or

$$\frac{m}{m_{00}^*} = 1 + \frac{P^2}{3} \left[\frac{2}{E_0^*} + \frac{1}{E_0^* + \Delta_0} \right] \dots\dots\dots [2:34]$$

and

$$P^2 = \frac{E_0^*(E_0^* + \Delta_0)}{(E_0^* + 2/3\Delta_0)} \left(\frac{m}{m_{00}^*} - 1 \right) \dots\dots\dots [2:35]$$

Equation [2:33] can be rewritten as

$$(E - ak^2)(E - ak^2 + E_0^*) = ak^2 P^2 \frac{E_0^* + 2/3\Delta_0}{E_0^* + \Delta_0} \left[\frac{1 + \frac{E - ak^2}{E_0^* + 2/3\Delta_0}}{1 + \frac{E - ak^2}{E_0^* + \Delta_0}} \right]$$

and replacing [2:35] in above

$$(E - ak^2)(E - ak^2 + E_0^*) = ak^2 E_0^* \left(\frac{m}{m_{00}^*} - 1 \right) \left[\frac{1 + \frac{E - ak^2}{E_0^* + 2/3\Delta_0}}{1 + \frac{E - ak^2}{E_0^* + \Delta_0}} \right]$$

Under the approximation that $E - ak^2 < E_0^* + 2/3\Delta_0$, which is true for

most III-V materials when doping levels are not excessive, the above equation reduces to

$$(E - ak^2)(E - ak^2) + E_0^* - aE_0^*\left(\frac{m}{m_{00}^*} - 1\right)k^2 = 0$$

which is now independent of Δ_0 . Expanding the above and solving for $(E - ak^2)$ gives

$$E - ak^2 = -\frac{E_0^*}{2} \pm \frac{1}{2} \left\{ E_0^{*2} + 4aE_0^*\left(\frac{m}{m_{00}^*} - 1\right)k^2 \right\}^{\frac{1}{2}}$$

For the (000) conduction band $E = 0$ when $k = 0$ and therefore the positive root is chosen. The model for the conduction band is thus

$$E = ak^2 + \frac{E_0^*}{2} \left[\left\{ 1 + \frac{4a}{E_0^*} \left(\frac{m}{m_{00}^*} - 1 \right) k^2 \right\}^{\frac{1}{2}} - 1 \right] \dots\dots\dots [2:36]$$

It is now possible to express the angle at rotation and the carrier concentration in terms of the band parameters E_0^* and m_{00}^* . In the sections which follow the final forms of the equations used in the analysis of the experimental data will be developed.

v) Statistical Free Carrier Faraday Rotation Relation:

Using equation [2:36] the following derivatives are found

$$\frac{\partial E}{\partial k_x} = 2ak_x + 2ak_x \left(\frac{m}{m_{00}^*} - 1 \right) A$$

$$\frac{\partial E}{\partial k_y} = 2ak_y + 2ak_y \left(\frac{m}{m_{00}^*} - 1 \right) A$$

$$\frac{\partial^2 E}{\partial k_x \partial k_y} = - \frac{8a^2}{E_0^*} k_x k_y \left(\frac{m}{m_{00}^*} - 1 \right)^2 A^3$$

$$\frac{\partial E}{\partial k_y} \frac{\partial^2 E}{\partial k_x \partial k_y} = - 16a^3 k_x k_y^2 \left(\frac{m}{m_{00}^*} - 1 \right)^2 A^3 - \frac{16a^3}{m_0^*} k_x k_y^2 \left(\frac{m}{m_{00}^*} - 1 \right)^3 A^4$$

$$\frac{\partial^2 E}{\partial k_y^2} = 2a + 2a \left(\frac{m}{m_{00}^*} - 1 \right) A - \frac{8a^2}{m_0^*} k_y^2 \left(\frac{m}{m_{00}^*} - 1 \right)^2 A^3$$

$$\frac{\partial E}{\partial k_x} \frac{\partial^2 E}{\partial k_y^2} = 4a^2 k_x + 8a^2 k_x \left(\frac{m}{m_{00}^*} - 1 \right) A + 4a^2 k_x \left(\frac{m}{m_{00}^*} - 1 \right)^2 A^2 - 16a^3 k_x k_y^2 \left(\frac{m}{m_{00}^*} - 1 \right)^2 A^3$$

$$- \frac{16a^3}{E_0^*} k_x k_y^2 \left(\frac{m}{m_{00}^*} - 1 \right)^3 A^4$$

where $A = \left\{ 1 + \frac{4a}{E_0^*} \left(\frac{m}{m_{00}^*} - 1 \right) k^2 \right\}^{-\frac{1}{2}}$ and hence

$$\left[\frac{\partial E}{\partial k_y} \frac{\partial^2 E}{\partial k_x \partial k_y} - \frac{\partial E}{\partial k_x} \frac{\partial^2 E}{\partial k_y^2} \right] = - 4a^2 k_x \left[1 + \left(\frac{m}{m_{00}^*} - 1 \right) A \right]^2$$

and

$$\frac{\partial E}{\partial k_x} \left[\frac{\partial E}{\partial k_y} \frac{\partial^2 E}{\partial k_x \partial k_y} - \frac{\partial E}{\partial k_x} \frac{\partial^2 E}{\partial k_y^2} \right] = - 8a^3 k_x^2 \left[1 + \left(\frac{m}{m_{00}^*} - 1 \right) A \right]^3$$

This is inserted into [2:27] and since the constant energy surfaces involved here are spherical, the co-ordinates may be converted into spherical co-ordinates (k, θ, ϕ) and the integration over θ and ϕ may be performed. Here then $d^3k = k^2 \sin \phi dk d\phi d\theta$ and $k_x^2 = k^2 \sin^2 \phi \cos^2 \theta$, and the integral in the Faraday relation is given by

$$I_1 = - 8a^3 \int_0^\infty \int_0^\pi \int_0^{2\pi} \frac{\partial f_0}{\partial E} G k^4 \sin^3 \phi \cos^2 \theta dk d\phi d\theta$$

where

$$G = \left[1 + \left(\frac{m}{m_{00}^*} - 1 \right) A \right]^3$$

$$= - 8\pi a^3 \int_0^\infty \int_0^\pi \frac{\partial f_0}{\partial E} G k^4 \sin^3 \phi dk d\phi$$

$$= - \frac{32\pi a^3}{3} \int_0^\infty \frac{\partial f_0}{\partial E} G k^4 dk$$

and using the definition for f_0 given previously

$$I_1 = \frac{32\pi a^3}{3kT} \int_0^\infty \frac{k^4 \left[1 + \left(\frac{m}{m_{00}^*} - 1 \right) \left\{ 1 + \frac{4a}{E_0^*} \left(\frac{m}{m_{00}^*} - 1 \right) k^2 \right\}^{-\frac{1}{2}} \right]^3 dk}{2 + \exp \left\{ \frac{E - E_{F0}}{kT} \right\} + \exp \left\{ \frac{E_{F0} - E}{kT} \right\}} \dots \dots \dots [2:37]$$

Under the condition of spherical constant energy surfaces, the carrier concentration for the (000) conduction band is given by

$$n_0 = \frac{2}{8\pi^3} \cdot 4\pi \int_0^\infty f_0 k^2 dk$$

or
$$n_0 = \frac{I_1'}{\pi^2} \dots \dots \dots [2:38]$$

and from [2:37]

$$\theta = \frac{60e^3 a^3 t B}{\pi^5 h^4 C^3 \epsilon_0 \eta} \left(\frac{I_1'}{kT} \right) \lambda^2 \dots \dots \dots [2:39]$$

where $I_1' = \int_0^\infty \frac{k^4 \left[1 + \left(\frac{m}{m_{00}^*} - 1 \right) \left\{ 1 + \frac{4a}{E_0^*} \left(\frac{m}{m_{00}^*} - 1 \right) k^2 \right\}^{-\frac{1}{2}} \right]^3 dk}{2 + \exp \left\{ \frac{E - E_{F0}}{kT} \right\} + \exp \left\{ \frac{E_{F0} - E}{kT} \right\}}$

and
$$I_2' = \int_0^\infty \frac{k^2 dk}{1 + \exp \left\{ \frac{E - E_{F0}}{kT} \right\}}$$

and in this case the Faraday effective mass is given by

$$\frac{m_{oF}^*}{m} = \left[\frac{3kT I_2'}{2a I_1'} \right]^{\frac{1}{2}} \dots\dots\dots [2:40]$$

The use of equations [2:38], [2:39] and [2:40] in the analysis of data will be further discussed in chapter 4. The integrals in these equations must be evaluated and this can be done either by numerical means or by converting the integrals to Fermi integrals. Tables of Fermi integrals were calculated in this laboratory by Coderre¹⁸ for a wide range of Fermi levels. For this reason a density of states equation for the case of spherical constant energy surfaces and a Kane-type conduction band has been derived by using equations [2:36] and [2:38]. This relation has been previously given by Ehrenreich⁵⁸ but his equation differs slightly from the one given here. This is probably due to the different forms of Kane equation chosen. In the next section a brief outline of the derivation of the density of states equation will be given. Equation [2:39] has also been converted into one involving generalized Fermi-Dirac integrals by other researchers⁵⁹ and tables of these integrals are available. However, since numerical integration is performed quite easily with the high speed I.B.M. computer available in this laboratory, the equations are used as shown above.

vi) Density of States Equations:

For the case of spherical energy surfaces and arbitrary band shapes, the carrier concentration is given by equation [2:38]. The Fermi integrals are defined by

$$(kT)^{(q+1)} F_q \left(\frac{E_{Fi}}{kT} \right) = \int_0^{\infty} f_0 E^q dE \dots\dots\dots [2:41]$$

Hence if for the (000) conduction band, the carrier concentration equation is rewritten as

$$n_0 = \frac{1}{\pi^2} \int_0^{\infty} f_0 k^2 \frac{dk}{dE} dE$$

then using the Kane equation [2:36] the term $k^2 \frac{dk}{dE}$ must be expressed in terms of E alone. On rearranging [2:36] and solving for k^2 one gets

$$k^2 = \pm \left[\frac{2E}{a} + \frac{E_0^*}{a} \left(\frac{m}{m_{00}^*} \right) \right] \pm \frac{E_0^*}{2a} \left(\frac{m}{m_{00}^*} \right) \left[1 - \frac{4E}{E_0^*} \left(\frac{m_{00}^*}{m} \right) \left(\frac{m_{00}^*}{m} - 1 \right) \right]^{\frac{1}{2}}$$

and for the (000) band at $E = 0$, $k = 0$. Therefore the -ve root is chosen. Furthermore when $E = 1\text{eV}$ the factor $\frac{4E}{E_0^*} \left(\frac{m_{00}^*}{m} \right) \left(\frac{m_{00}^*}{m} - 1 \right) \approx 0.4$ for GaAs and 0.3 for InSb. The square root may thus be expanded using the binomial theorem and after some manipulation

$$k^2 = \frac{E}{a} \left(\frac{m_{00}^*}{m} \right) \left\{ 1 + \left(\frac{E}{E_0^*} \right) \left(\frac{m_{00}^*}{m} - 1 \right)^2 + 2 \left(\frac{E}{E_0^*} \right)^2 \left(\frac{m_{00}^*}{m} \right) \left(\frac{m_{00}^*}{m} - 1 \right)^3 \right. \\ \left. + 5 \left(\frac{E}{E_0^*} \right)^3 \left(\frac{m_{00}^*}{m} \right)^2 \left(\frac{m_{00}^*}{m} - 1 \right)^4 + 14 \left(\frac{E}{E_0^*} \right)^4 \left(\frac{m_{00}^*}{m} \right)^3 \left(\frac{m_{00}^*}{m} - 1 \right)^5 \right\}$$

from the above relation the terms $2k \frac{dk}{dE}$ and k can then be found and it is found that

$$2k^2 \frac{dk}{dE} = \left[\frac{m_{00}^*}{m} \cdot \frac{1}{a} \right]^{3/2} E^{1/2} \left\{ 1 + \left(\frac{5}{2} - 5 \frac{m_{00}^*}{m} \right) \left(\frac{E}{E_0^*} \right) + \left(\frac{7}{8} - \frac{21}{2} \frac{m_{00}^*}{m} \right) \left(\frac{E}{E_0^*} \right)^2 \right. \\ \left. - \left(\frac{1}{4} + 3 \frac{m_{00}^*}{m} \right) \left(\frac{E}{E_0^*} \right)^3 \right\}$$

and replacing the carrier concentration integral

$$n_0 = \frac{1}{2\pi^2} \left[\frac{m_{00}^*}{m} \frac{kT}{a} \right]^{3/2} \left\{ F_{1/2} \left(\frac{E_{F0}}{kT} \right) + \left(\frac{kT}{E_0^*} \right) \left(\frac{5}{2} - 5 \frac{m_{00}^*}{m} \right) F_{3/2} \left(\frac{E_{F0}}{kT} \right) \right. \\ \left. + \left(\frac{kT}{E_0^*} \right)^2 \left(\frac{7}{8} - \frac{21}{2} \frac{m_{00}^*}{m} \right) F_{5/2} \left(\frac{E_{F0}}{kT} \right) \right. \\ \left. - \left(\frac{kT}{E_0^*} \right)^3 \left(\frac{1}{4} + 3 \frac{m_{00}^*}{m} \right) F_{7/2} \left(\frac{E_{F0}}{kT} \right) \right\} \dots \dots \dots [2:42]$$

As has been mentioned before this equation differs only slightly from that developed by Ehrenreich in that the coefficient of $F_{7/2}$ is different.

For the III-V materials dealt with in this thesis, however, this difference is hardly detectable.

For the case of non-spherical energy surfaces and parabolic bands the density of states equation quoted in the literature⁴² is

$$n_i = \frac{M}{2\pi^2} \left(\frac{m_{id}^*}{m} \right) \cdot \left(\frac{kT}{a} \right)^{3/2} F_{\frac{1}{2}} (E_{Fi}/kT) \dots\dots\dots [2:43]$$

where M is the multiplicity of these bands and m_{id}^* is found from [1:8].

CHAPTER 3

E X P E R I M E N T A T I O N

i) Introduction:

By 1964, only a few experimental values^{60,61} for the effective mass of conduction electrons in mixed III-V crystals had been given and other values had been obtained through empirical calculations. These calculations¹⁰⁴ showed that the bottom of the conduction band effective mass varied smoothly with composition and, like the fundamental gap, this variation showed a minimum at a composition of about 50%. It was therefore of interest to measure this effective mass using the most direct means so that the calculated variation with composition could be compared with the experimentally obtained values. This project was originally focussed on measuring the effective mass of electrons in alloys by means of the free carrier Faraday effect and although measurements were to be made on the III-V compound components of these alloys these data would only serve as a complement to the alloy results. It will be seen, however, that some interesting results were obtained from the measurements on InSb and GaSb.

Since the alloys were not available commercially it was necessary to grow the material in this Laboratory. Most of the detailed investigation into preparation procedures was done here by Coderre, but it is a group policy that every member should contribute to this aspect of the research.

The alloys with which the author was concerned were those of the $\text{In}_{1-x}\text{Ga}_x\text{Sb}$ system. A few details about the preparation of these materials will be given later.

In order that the equations in Chapter 2 could be used with as few assumptions as possible it was necessary to study other effects besides free carrier Faraday rotation. For instance, the carrier concentration could be measured by observing the variation of the Hall coefficient as a function of the magnetic field and also an estimate of the position of the Fermi level could be made from thermoelectric power measurements. Other effects such as optical absorption in the intrinsic and free carrier wavelength region were also studied so that the amount of absorption could be estimated.

The general procedure which was followed on each specimen was first to prepare the specimen for the optical work by lapping and polishing. After this the Faraday, Hall, thermoelectric power and other optical experiments were carried out. Finally the specimen were ground to a powder and X-ray powder photographs were taken in order to determine the composition of each specimen.

In the following sections the steps in the procedure will be outlined in more detail and the equipment used for each measurement will be described.

ii) Preparation of Specimen:

It is possible to grow $\text{In}_{1-x}\text{Ga}_x\text{Sb}$ specimen by the directional freeze technique described by Woolley et al.^{26,62}. In this method the material, which has been sealed under vacuum in a quartz capsule, is placed in a furnace which has a temperature gradient such as that shown in fig. (3; 1(a)). The control temperature of the furnace is slowly lowered and due to the gradient the material begins to freeze from one end. The rate of freezing is critical and a sensitive temperature control system is required. Because of the very low diffusion rates in the materials the directional freeze method requires very long cooling times and ingots were usually grown over a period of three months. It was found, however, that in many cases equilibrium had not been reached and this resulted in multiphase material. This undesirable result was attributed to constitutional supercooling. One method of eliminating this effect was to increase the temperature gradient of the furnace but this is not practical since to attain the desired gradient for some alloys systems one end of the furnace would have to be over 1200°C which is close to the melting point of quartz as well as above the specified operating temperature of the Canthal wire used in the furnace winding. Consequently another method was tried. This is the step-freeze method and is an adaptation of the well known horizontal Bridgman technique.

The furnace profile used in this method is shown in fig. (3; 1(b)). The steep temperature gradient is attained by using water cooled baffles.

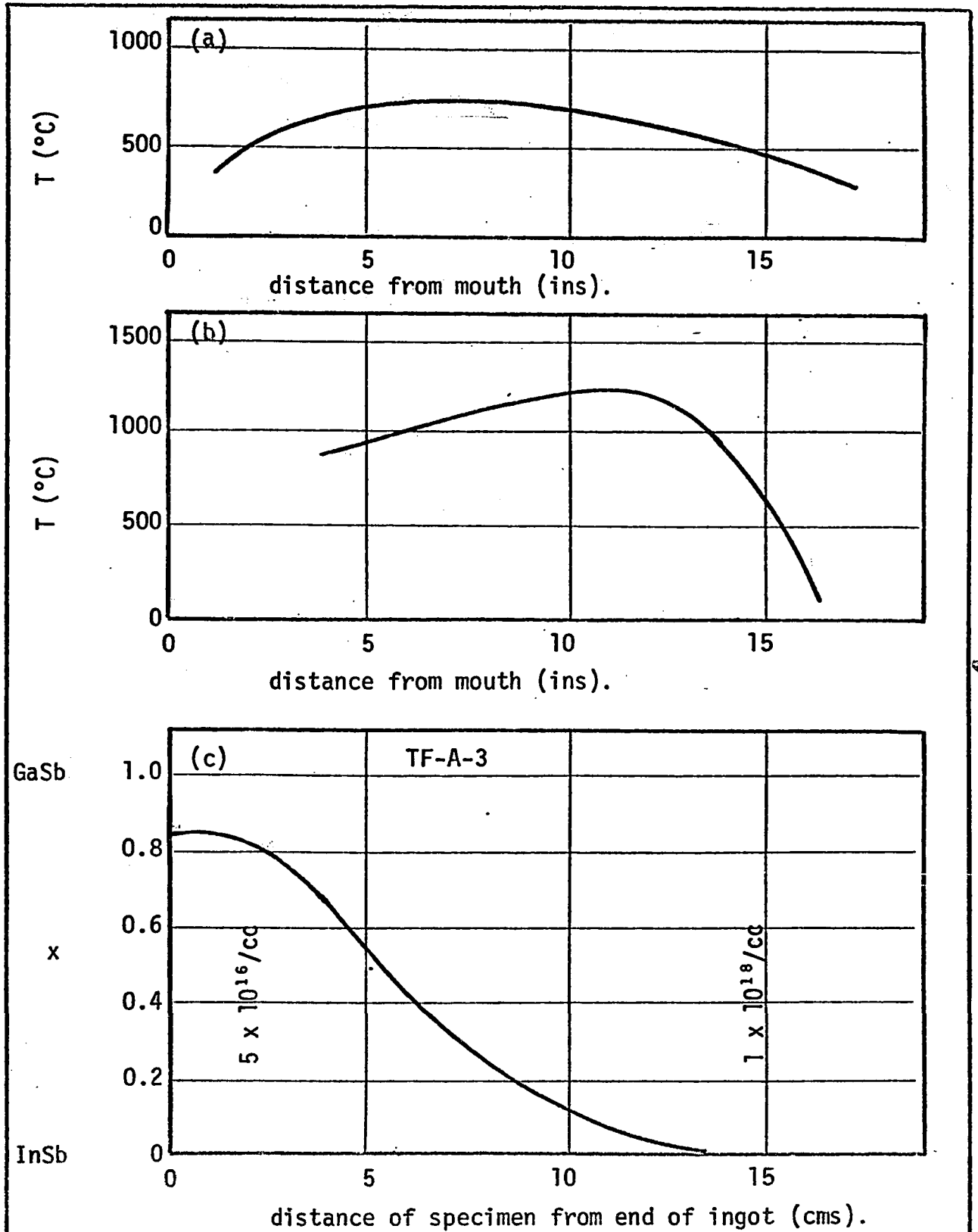


Fig. (3:1): Typical curves in specimen preparation.

The hot zone of the furnace need only be above the highest melting point of the two compounds. For the $\text{In}_{1-x}\text{Ga}_x\text{Sb}$ systems the melting points are about 525°C for InSb and 710°C for GaSb and hence the hot zone is usually kept at about 900°C . Hence in this method the furnace profile is not changed and the specimen is pulled through the step by an external driving mechanism. Here the temperature control is not so critical. In the first attempts no temperature stabilising system was used at all and using growth times of about one month very good single phase material was obtained over the whole composition range. This system can thus be grown relatively easily using this method. In fact growth times of only 15 days for 15cm. ingots are used now and no temperature control is needed. Growing specimen at 1 cm./day results in ingots of uniform cross-section and this is of advantage in optical work.

In fig. (3; 1(c)) the variation of composition with length is shown for a typical ingot which was grown using the step-freeze technique and starting from a 50-50 mole percent mixture of the compounds. The composition was found using standard X-ray powder photograph techniques. From the resolution of the large angle back-reflected lines on these photographs the homogeneity of these specimen was seen to be very good and thus the lattice parameter could be determined to within 0.5%. The determination of the composition from the lattice parameter was dependent on published data of the variation of lattice parameter with composition²⁶, and it is estimated that compositions were found to within 1%.

Some preliminary values for the doping level in the ingot are also shown in fig. (3; 1(c)). This level of doping was attained by adding one milligram of Te to the 50 gram mixture of commercial polycrystalline InSb (approximately $3 \times 10^{22}/\text{m}^3$ n-type carriers) and polycrystalline GaSb prepared in this laboratory (roughly $10^{23}/\text{m}^3$ p-type carriers).

The measurements on $\text{In Sb}_{1-x} \text{As}_x$ specimens were made on material prepared in this laboratory by Coderre and the methods of preparation are described elsewhere¹⁸. There are still many problems with the growing of these crystals but nevertheless the specimens which were obtained were homogeneous to about 1%.

The GaSb specimen used were supplied by Dr. A. Strauss of the Lincoln Laboratories, M.I.T. and had been used previously in magneto-resistance work⁷⁴. The samples were n-type single crystals and were cut from ingots which were pulled from a melt which consisted of Te and p-type GaSb having hole concentrations of the order of $2 \times 10^{23}/\text{m}^3$.

The optical specimen were obtained from cross-sectional slices of the ingots. Since electrical and thermal measurements were to be made as well, the slices were cut to be roughly rectangular and were on the average 1cm. x 2-3 mms. in dimensions. Thus the cross-sectional area was convenient for optical work and the length to width ratio was adequate for the (simple) Hall effect measurements. These rectangular slices were ground to roughly 150 microns using coarse alumina powder. The two surfaces were then mechanically polished using 1 micron alumina powder. In this way the scattering of radiation was reduced and the transmitted intensity was increased.

iii) The Magneto-optical System:

In discussions with Dr. M. Cardona during his visit to this laboratory in 1964, it was pointed out that one of the most difficult aspects of magneto-optical experiments is the aligning of the optical system. In order to facilitate the alignment, therefore, the mirror, polarizer and detector holders were designed to give as many degrees of freedom as possible. All the components of the optical system could be positioned by means of coarse and fine adjustment controls on the holders. In fig. (3:2), the details of the holders are shown, (a), together with the mirror supports, (b), and the specimen mount, (c). In figure (3:3), the detector and the final focussing mirror system, (a), and the analyser support, (b), are shown. The polariser mounting is the same as that for the analyser except that no external drive mechanism is attached. Wherever possible non-magnetic materials like brass, aluminum and stainless steel were used in the construction of all the components of the optical system.

In order to insure that the optical system was rigid so that after alignment all the components remained fixed, the mirrors, polarisers, sample holder and detector were suspended from a rigid frame. A schematic of the assembled system is shown in figure (3:4) and is basically the same as that used by previous workers^{63,64}.

The monochromator is a Perkin-Elmer double pass model. It can be fitted with a NaCl or a KBr prism thus giving monochromatic radiation in

Fig. (3:2(a)): Optical holder.

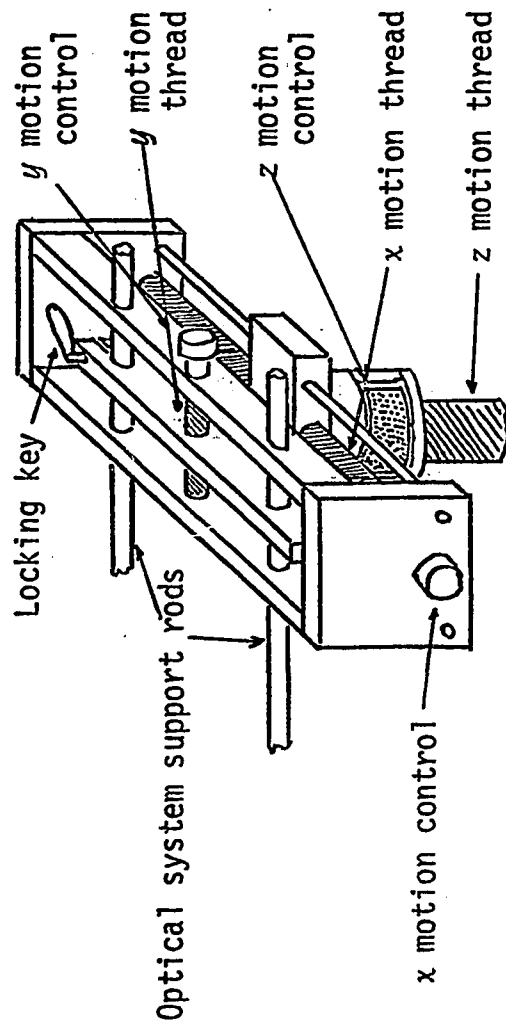


Fig. (3:2(c)): Specimen holder.

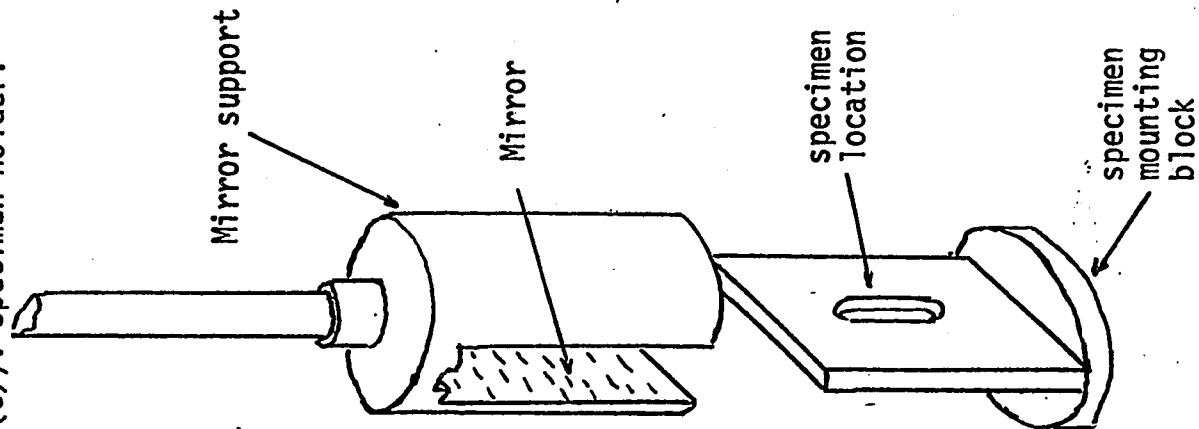


Fig. (3:2(b)): Mirror support.

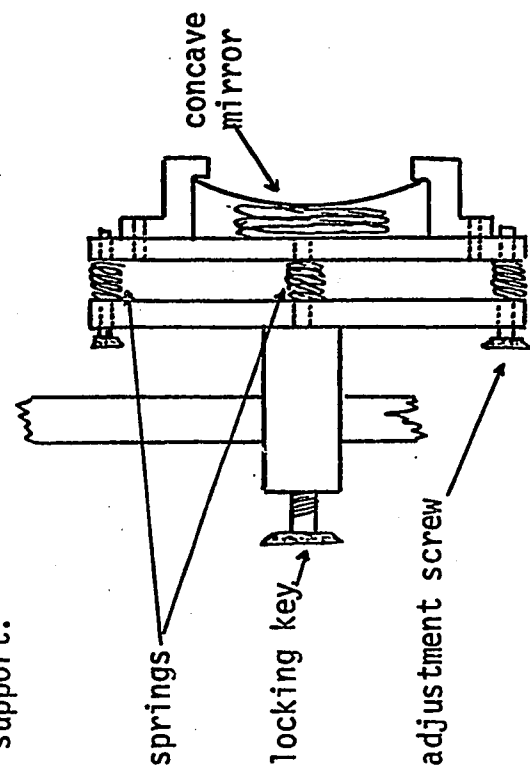


Fig. (3:3(a)) Detector mounting.

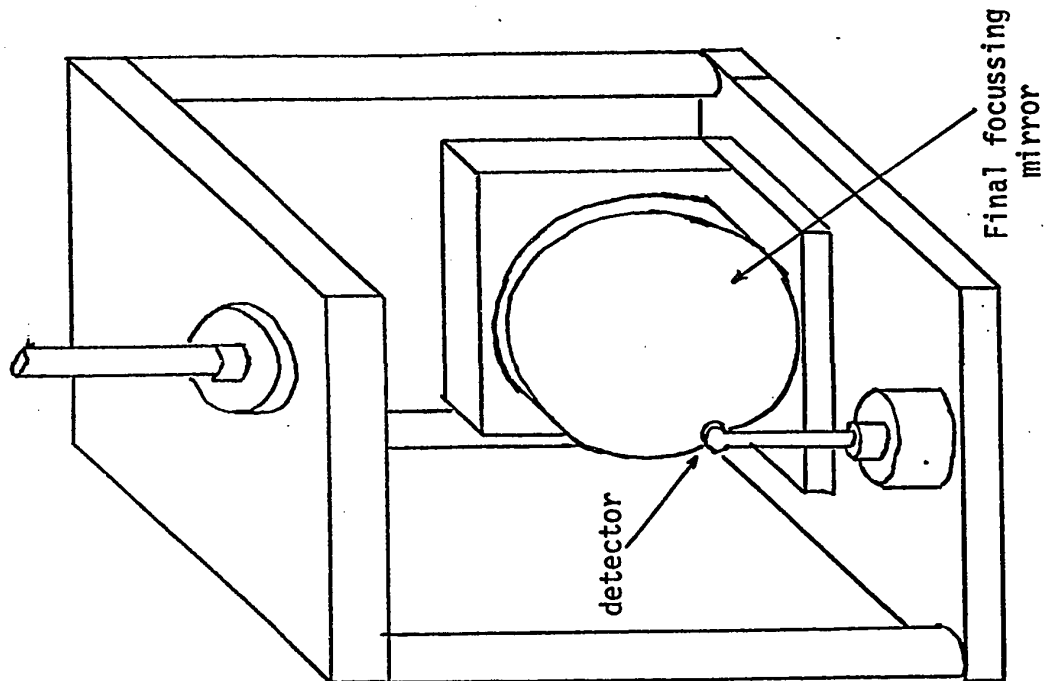
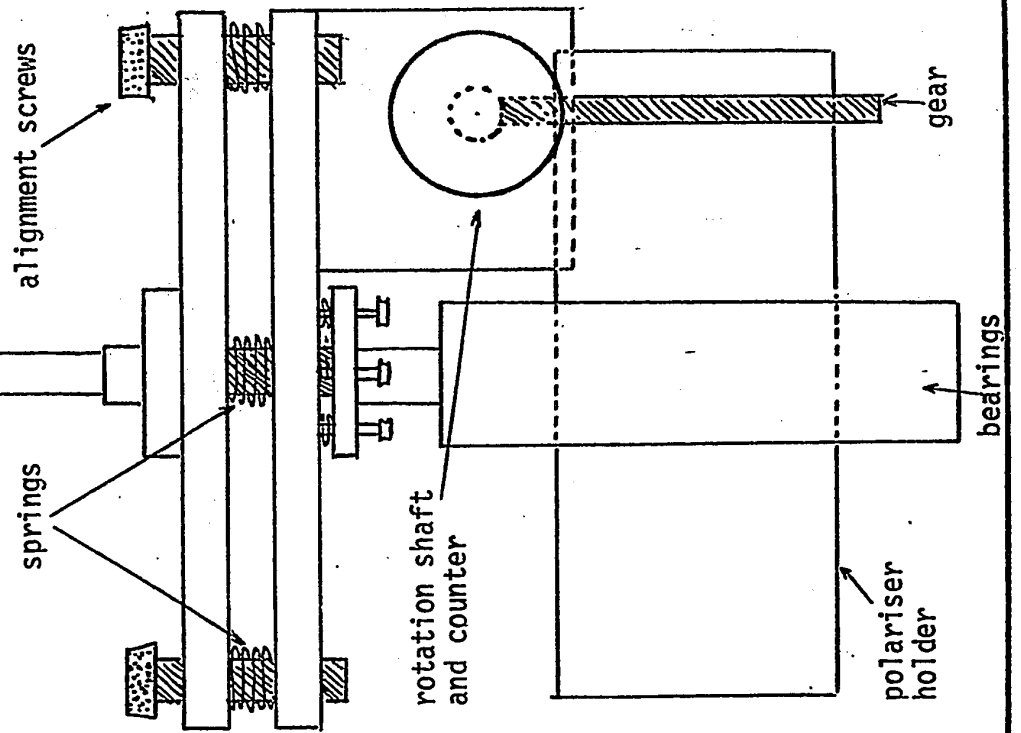


Fig. (3:3(b)): Analyser holder.



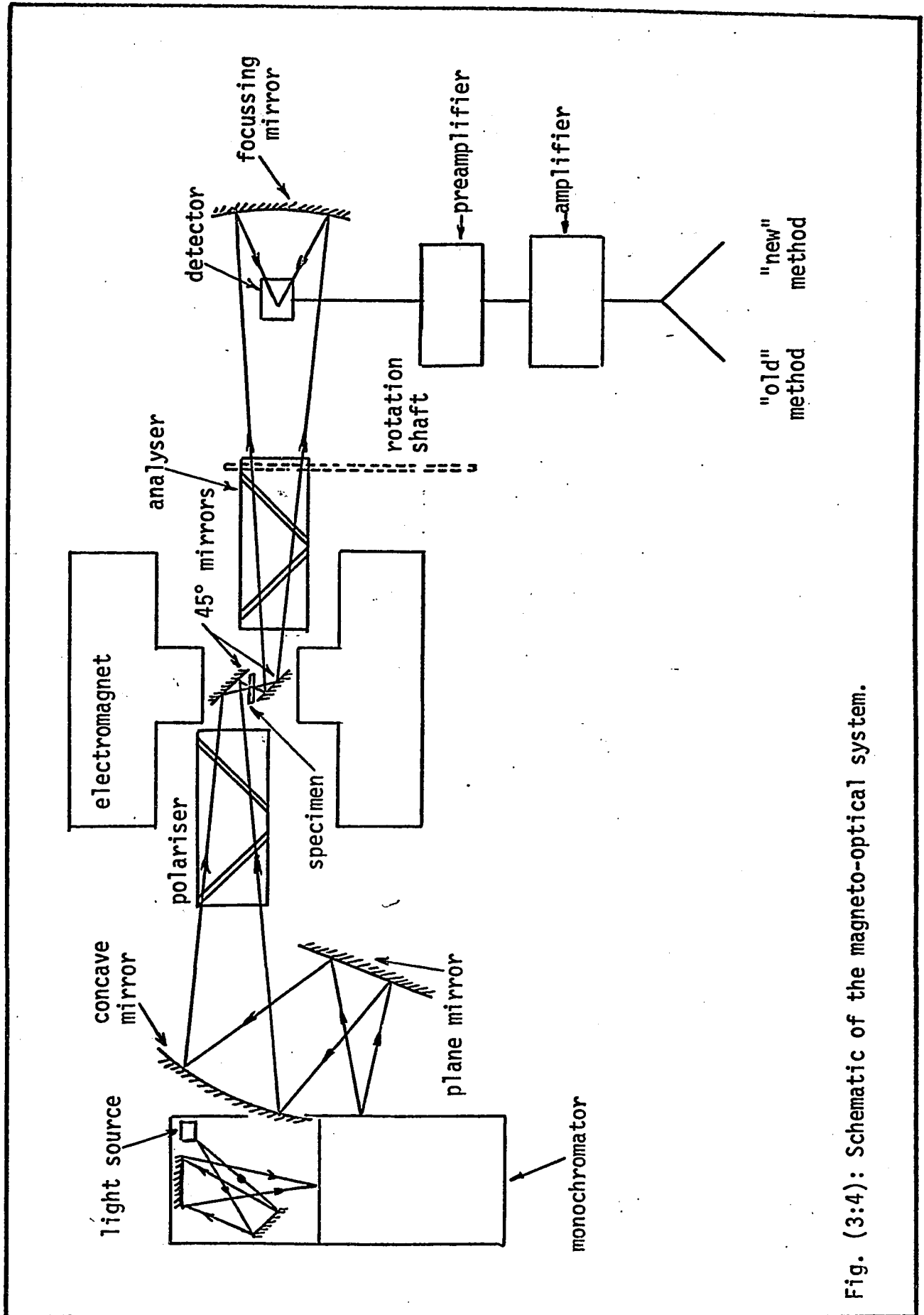


Fig. (3:4): Schematic of the magneto-optical system.

the 2 to 25 micron range. In order to facilitate amplification and to reduce noise due to stray light and fluctuations in the line voltage, the radiation is chopped at 12.5c.p.s. before being passed a second time through the prism. Mechanical contacts fixed to the chopper shaft are used to rectify the amplified signal.

The source is a Nernst filament powered by a regulated 110 VAC supply. The filament is capable of radiating about 100 watts of power at 100 VAC and can readily be used for the wavelength range given above.

The detector is a Perkin-Elmer thermocouple with a KBr window. The connection between the detector and the preamplifier is made as short as possible to reduce noise.

The wavelength of the radiation from the monochromator can be changed by rotating a Littrow mirror which is set directly behind the prism. The wavelength drum on the monochromator is graduated in "number of turns". In order to calibrate the drum in terms of wavelength, filters of different materials are used. From a number of well-known absorption bands in these materials, the wavelength and the drum reading can be correlated. For the wavelength range under consideration, 2 to 25 microns, suitable materials are benzene, polystyrene, chloroform, 1-2-4trichlorobenzene and FeCO_3 . The atmospheric CO_2 and moisture vapour lines can be used. A complete listing of the absorption bands for monochromator calibration from 2 to 16 microns is given by Plyler et al.⁶⁵. The calibration curves which were obtained for the NaCl and the KBr prisms are shown in figure (3:5).

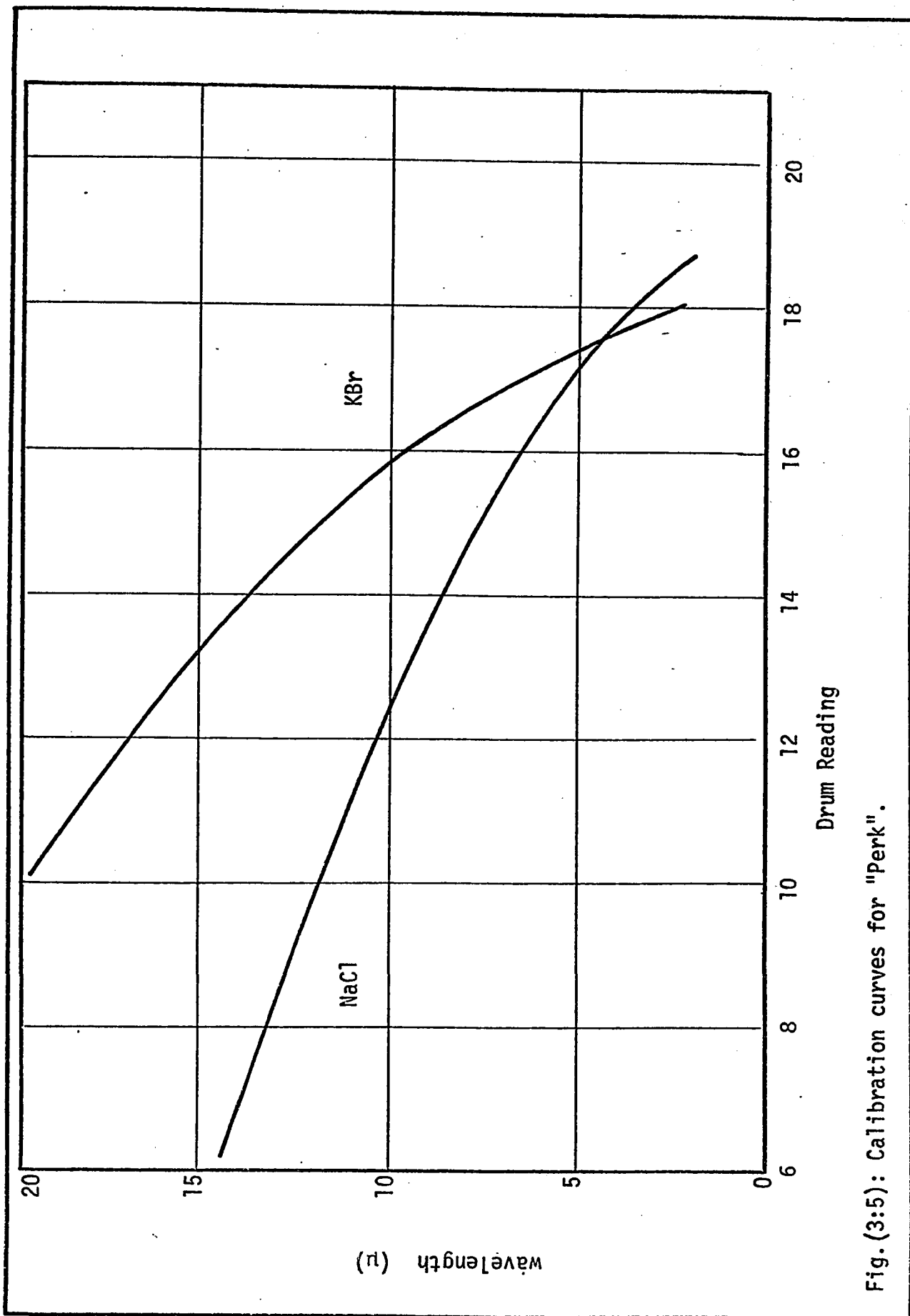


Fig. (3:5): Calibration curves for "Perk".

In order to keep the optical system as simple as possible it was decided to use linear transmission polarisers such as the pile-of-plates type. There are numerous materials which can be used for these polarisers. A listing of these is given by Palik⁶⁶. Initially the author had tried thin Mylar dielectric films (commercially known as Saran wrap). This proved to be only moderately successful and could be used solely in the 2 to 6 micron range. Here about 60% polarisation was attained for a "pile" of 4 films. Also since the Brewster angle is approximately 70° these polarisers tend to be rather bulky and so this material is not too practical. The polariser which was eventually used was the Beckmann silver chloride polariser. Although only about 30% of the incident radiation is transmitted by these polarisers they are suitable for use up to 20 microns without too much difficulty. One precaution which must always be taken when dealing with AgCl is that this material is sensitive to ultra-violet radiation and blackens after some exposure. The amount of u.v. in the room must therefore be kept to a minimum. It has been reported recently, however, that these plates may be restored to good condition by a lapping process. The Beckmann polariser consists of two sets of differently stacked plates and so the beam refracted by one set is refracted back onto the optic axis by the other set of plates. This is required for the method of measurement used here since the analyser is rotated. The driving mechanism of the analyser can be operated manually or by a motor drive which rotates the analyser at a rate of approximately two revolutions per hour.

The Newport magnet which was used, was capable of giving fields of 0.75 w/m^2 at a pole gap of 1.25". The field strength was measured with a Rawson rotating coil gaussmeter. It is estimated that the accuracy of the field measurement is better than 1%. Since the cross-sectional size of the samples is generally less than 0.3 cms² the inhomogeneity of the magnetic field need not be considered.

In order to reduce the intensity lost by the radiation along the optical path, the image of the exit slit of the monochromator is focussed on the specimen by a concave mirror which has a focal length, f , of 30cms.

The optimum condition was attained with a $2f:2f$ configuration of object and image distances. In this way the beam is slowly converging and hence hardly any intensity is lost at the aperture of the polariser. The light is rendered parallel to the magnetic field by using two small auxiliary mirrors placed at a 45° angle to the optical path. After passing through the analyser the radiation is focussed by a very short focal length concave mirror onto the detector. The resulting chopped signal is preamplified, amplified and rectified. The output DC voltage can then be displayed on a Philips Chart Recorder or connected to a bridge circuit which will be described in the next section.

iv) Measurement Procedure:

Two methods of measuring the Faraday rotation θ were used. In the first the output from the amplifier was connected in series with the Philips recorder and the secondary coil of an output transformer. The primary coil was connected to a circuit which was used to superimpose marks on the recorder trace as the analyser was rotated. This marker unit is shown in figure (3:6). The driving motor rotated at $\frac{1}{2}$ rev/min. and turned the flywheel at 1 rev/min. There were two small holes on the circumference of the flywheel. These holes permitted light to activate the photocell and hence current flowed through the relay windings. A voltage was thus applied across the primary coil and the change in flux in the transformer caused the superimposed marks on the recorder trace. Since there was a 2:25 gear ratio between the analyser and the analyser drive shaft there were 50 such marks for every full rotation of the analyser. The spacing between two marks thus corresponded to 7.2° of rotation of the analyser. The amount of slippage and backlash between all the gears could be tested by running a number of traces of full revolutions in the forward and reverse directions of the motor drive and comparing the traces and the positions of the marks. There was a slight difference in intensity from one trace to another but this was only attributed to fluctuations in the source since the positions of these marks relative to the maxima and minima of the trace were always constant.

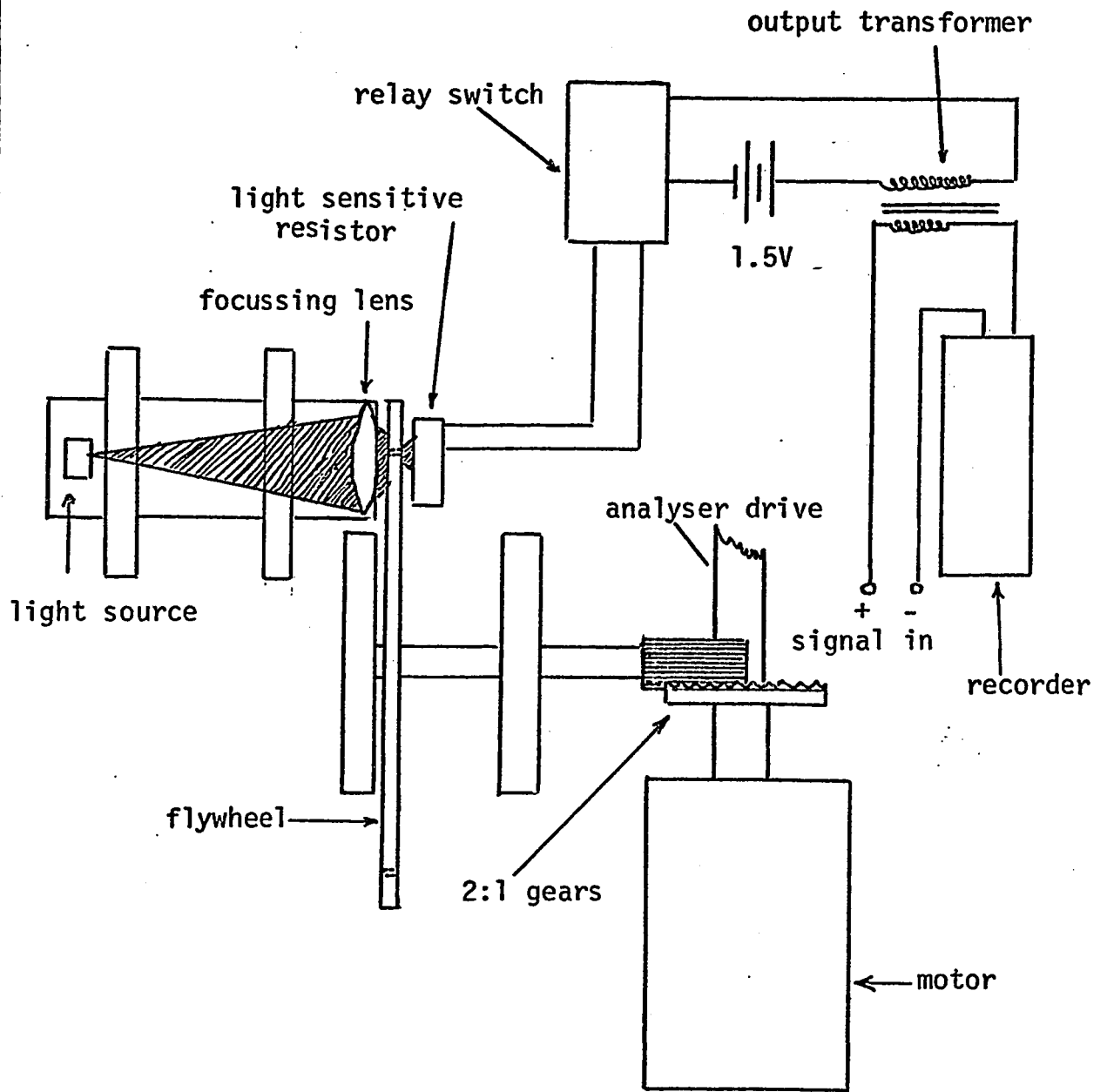


Fig. (3:6): Marker system

In the measurement of the Faraday rotation the magnetic field was set to the desired value and the monochromator to a wavelength well above the fundamental absorption region. The gain on the amplifier was adjusted to give full scale deflection when the polarised beam incident on the analyser and the analyser were in the parallel position. The zero balance on the amplifier was adjusted when this beam and the analyser were in the crossed position. The analyser was then motor driven through one full revolution and a complete output trace was obtained. The magnetic field was then reversed and the procedure was repeated. The intensity at each of the markers was read off for each trace and the traces were computer fitted by a least squares fit to a curve of the form.

$$y_i = y_0 + c \sin (\phi_{\pm} + x_i)$$

where $\pm$ corresponds to the two field directions. The Faraday rotation of the specimen is then given by

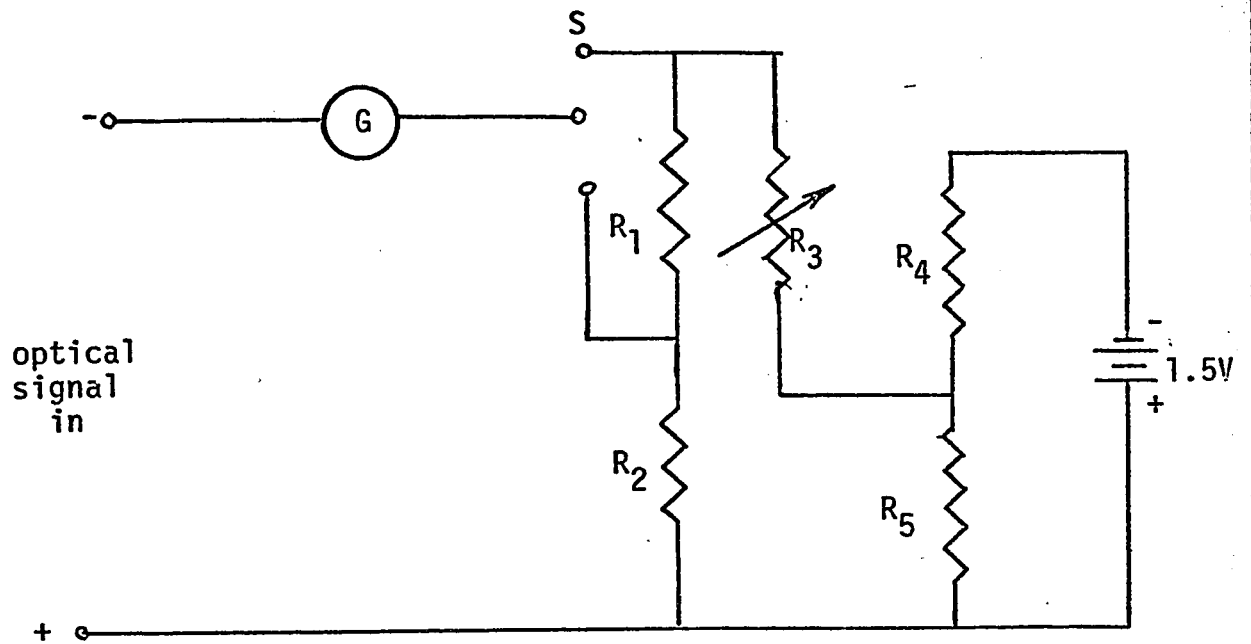
$$\theta = 0.25 (\phi_+ - \phi_-)$$

The results of these measurements will be shown in the next chapter.

This method is slow and rather tedious but gives an accurate result, since misalignment effects are averaged out. The accuracy attained by this method can be estimated from the standard deviation calculated in the curve

fitting program. In all cases it was found that the rotation was measured to better than 0.5° .

In the second method the amplifier output signal was connected in series with a sensitive galvanometer and a variable DC voltage supply. The circuit diagram is shown in figure (3:7). With the magnetic field applied and the analyser adjusted to give maximum transmittance, the variable DC voltage was adjusted until the galvanometer reading was zero, i.e., at this position the output signal and the DC voltage were equal in magnitude. The DC voltage was then reduced to half its value and the analyser was rotated until the galvanometer again read zero. The position ϕ_1 of half maximum transmission was recorded on a counter connected to the analyser rotation shaft. The magnetic field was reversed and a new value ϕ_2 obtained. The value of θ is given by $0.5 (\phi_1 - \phi_2)$. In order to average out misalignment effects, the values of all four half-maximum transmittance points in a full analyser rotation were found and a mean θ calculated. The position of half maximum transmittance was used since the amplifier signal varies most rapidly with the analyser angle at this point. This method of determining θ was much faster than the first and appeared to give very similar results. It is estimated that the values of θ obtained by this method were accurate to about 0.5° . This estimate was made by comparing the values obtained by both methods. This comparison is shown in fig. (4:10) in chapter 4.



G: Gavanometer

S: Single pole double throw switch

R_1 : 1000Ω

R_2 : 1000Ω

R_3 : 1000Ω potentiometer

R_4 : $1M\Omega$

R_5 : 100Ω

Fig. (3:7): Circuit diagram for "new" method.

1) Hall Effect Measurement:

The probe used in the electrical measurements was of the standard type. Only four contact points were used, two for the current which flowed along the length of the specimen and two to pick up the Hall voltage across the width of the specimen. The magnetic field is applied perpendicularly to these two directions. Since the specimen to be measured were in the shape of thin platelets, no strong spring devices could be used for making the contacts. In all cases, however, a good mechanical contact could be obtained by using gold wire of about 0.005" in diameter. The spring action of these wires was sufficient to obtain good contacts giving resistances of the order 200 ohms between the current leads and slightly less between the voltage leads. These resistances could be lowered considerably by spark welding the gold wire to the specimen and in general the values obtained were around 5 ohms. These contacts were found to be ohmic.

In order to calculate the carrier concentration from the Hall experiment the relation between the Hall coefficient, R_{Hi} , and the number of carriers, n_i , must be used. This relation is given by

$$R_{Hi} = \frac{r_i F_i}{n_i e} \dots\dots\dots [3:1]$$

For a single band which is designated by the subscript i as in Chapter 1. In equation [3:1] r_i is known as the Hall parameter and F_i is a geometric factor which depends on the shape of the constant energy

surfaces. The expression relating F_i to the shape of these surfaces is ⁶⁸

$$F_i = \frac{3K_i(K_i + 2)}{(2K_i + 1)^2} \dots\dots\dots[3:2]$$

where K_i is the same as used in [1:4] and [1:5] i.e. the ratio of the longitudinal to transverse effective masses.

More will be said concerning this formula later on. The Hall coefficient is related to measurable quantities by

$$R_{Hi} = \frac{tV_H}{IB}$$

where t is the specimen thickness, V_H is the Hall voltage, I is the current used and B is the magnetic field.

The thickness of the specimen was measured using a Mercer dial indicator which was graduated in 10 microns divisions. Numerous measurements were taken over the surface of the specimen and the results were averaged. In this way the thickness was measured to within 5 microns.

The current was measured with a potentiometer set up and the inaccuracies associated with this measurement were negligible. The magnitude of the magnetic field could be read off the field control panel. The accuracy given by the manufacturers was below 1%.

In order to eliminate errors due to the misalignment of the voltage leads, the Hall voltage at one field was measured in both field directions

and the results were combined as follows

$$(V_+)_{\text{measured}} = V_H + V_{\text{offset}} + V_{\text{magnetoresistance}}$$

$$(V_-)_{\text{measured}} = -V_H + V_{\text{offset}} + V_{\text{magnetoresistance}}$$

therefore $(V_+)_{\text{measured}} - (V_-)_{\text{measured}} = 2V_H$

Since the offset voltage and the voltage due to magnetoresistance depend on the current direction only.

The problem in calculating the carrier concentration using equation [3:1] is that generally F_i and r_i are not known.

If however the carriers can be associated with the (000) band only the problem is simplified in that the energy surfaces here can be treated as being spherical. Hence $m_{ol} = m_{ot}$, $K_o = 1$ and hence $F_o = 1$. The Hall parameter, r_i , depends on the predominant scattering mechanism. In the case of degenerate material for a single (000) band, $r_o \rightarrow 1$. For non-degenerate material $r_o \neq 1$ but it has been shown by Smith⁶⁸ that the one band Hall coefficient for a non-degenerate specimen in an infinite magnetic field is given by

$$R_\infty = \frac{1}{n_o e} \dots\dots\dots [3:3]$$

The procedure followed was thus to observe the variation of the Hall coefficient in increasing magnetic fields. The saturation value of R_{H0} was then taken to be R_{∞} and from equation [3:3] the carrier concentration, n_0 , was found.

Other problems which are encountered in the measurement of the carrier concentration are the sample size factor and the inhomogeneity of doping within a specimen. For an ideal Hall measurement using the straight-forward four probe system the length to width ratio should be at least three⁷⁰. This was roughly satisfied in all cases. To justify the use of standard Hall effect measurement on the thin optical specimen an experiment was carried out whereby one slice of an ingot was measured before any further cutting, grinding or polishing. The length to width ratio was of approximately 2:1 and the carrier concentration was found to be 2.34×10^{23} n-type carriers /m³. A very thin parallelopiped was cut from one edge of this slice and the length to width ratio of this specimen was 10:1. The carrier concentration found in this case was 2.08×10^{23} /m³. The remaining part of the original slice was then ground down to about 100 microns and mechanically polished. The length to width ratio was about 3:1 and the measured carrier concentration was again 2.08×10^{23} /m³. Although arriving at the same value as before is coincidental since there should be some difference due to experimental inaccuracies this experiment shows that standard Hall effect measurements can be made on the thin optical sample and that inhomogeneity of doping within the platelet must

be small.

The Hall effect measurements could therefore be carried out after the measurement of the Faraday effect. The high field technique described above was used and the results are given in the next Chapter.

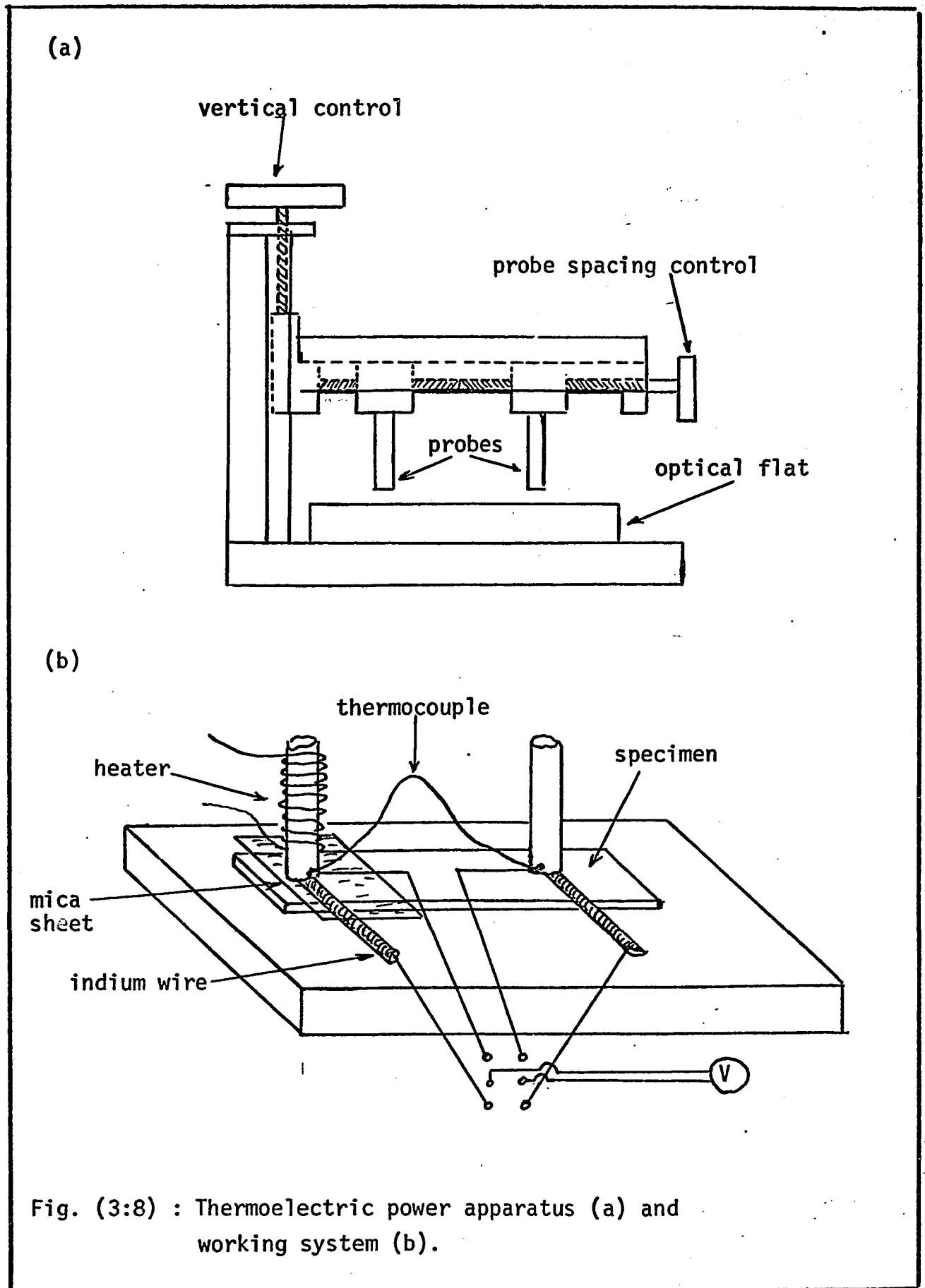
vi) Thermoelectric Power Measurements:

The conventional method of measuring the thermoelectric power by applying the heat source and the heat sink to the ends of the specimen could not be used here since the specimens were too thin and too brittle. A method was devised whereby the heat source and the heat sink are lowered onto the ends of the specimen which was mounted on a plate of optical quality glass. This method was found to prevent breakage. A diagram of the apparatus is given in figure (3, 8(a)). The horizontal screw permits adjustment of the spacing between the heat source and sink. The vertical screw lowers the probes onto the specimen.

The electrical system used in the measurement is shown in figure (3; 8(b)).

In order to achieve good electrical and thermal contacts between the specimen and the probes indium wire is used as indicated in (3; 8(b)). The voltage drop is thus measured across the indium wires and the temperature difference between the ends of the specimen is found using a chromel-alumel thermocouple. Electrical insulation between the one junction of the thermocouple and the indium probe is obtained by using thin mica sheets.

The variation of voltage drop with temperature difference was measured using a Hewlett Packard preamplifier. The results of these measurements will be given in the next Chapter.



vii) Optical Absorption Measurements:

The magneto-optical system was designed so as to allow measurement of the absorption edge in the specimens. The amount of energy transmitted at each wavelength was measured both with and without a specimen. The ratio of these measurements thus gives the absorbance of the specimen.

These measurements were carried out to determine the degeneracy of the specimen and also to estimate the magnitude of the extinction coefficient. A knowledge of the latter is required in the analysis of Faraday rotation data when multiple internal reflection corrections are to be made.

The results of these experiments are shown in the next Chapter.

CHAPTER 4

E X P E R I M E N T A L D A T A

i) Introduction:

In this chapter a systematic listing of the experimental data will be given. Several times in the past the author has wanted to reanalyse the raw data of previous work. This however has been hampered by the fact that some of the fundamental measurements necessary for a reanalysis had not been recorded. It is hoped that should it be necessary to reanalyse the present data at some future date, the basic measurement results will be easily obtained.

The data will be recorded under the following headings in the next sections;

Section (ii) - Measurement on the compounds

(a) InSb

(b) GaAs

(c) GaSb

(d) InAs

Section (iii) - Measurements on alloys

(a) $\text{InSb}_{1-x}\text{As}_x$

(b) $\text{In}_{1-x}\text{Ga}_x\text{Sb}$

The specimens will be numbered according to their appearance in this thesis. Where there may be some confusion in specimen numbering, i.e. where a specimen has been numbered differently elsewhere as in a publication or other thesis this will be clearly indicated here.

As has been mentioned in Chapter 3, two different methods for measuring the Faraday rotation were developed. The first method was to actually make a trace out of the output on the recorder and then to fit this trace with a computer using a least squares method. This will be referred to as the "OLD" method. The second way was to electrically balance the output voltage and to use a galvanometer null technique. This will be referred to as the "NEW" method. Table 4A indicates which method was used for each specimen.

Specimen number	Method	Specimen number	Method	Specimen number	Method
1	old	15	old	29	new
2	old	16	new	30	new
3	old	17	old	31	new
4	old	18	new	32	new
5	new	19	new	33	new
6	new	20	new	34	new
7	old	21	new	35	new
8	old	22	new & old	36	new
9	old	23	new	37	new
10	old	24	new	38	new
11	old	25	new	39	new
12	old	26	old	40	new
13	old	27	old	41	new
14	old	28	new	42	new

T A B L E 4A

ii) Measurements on the Compounds:

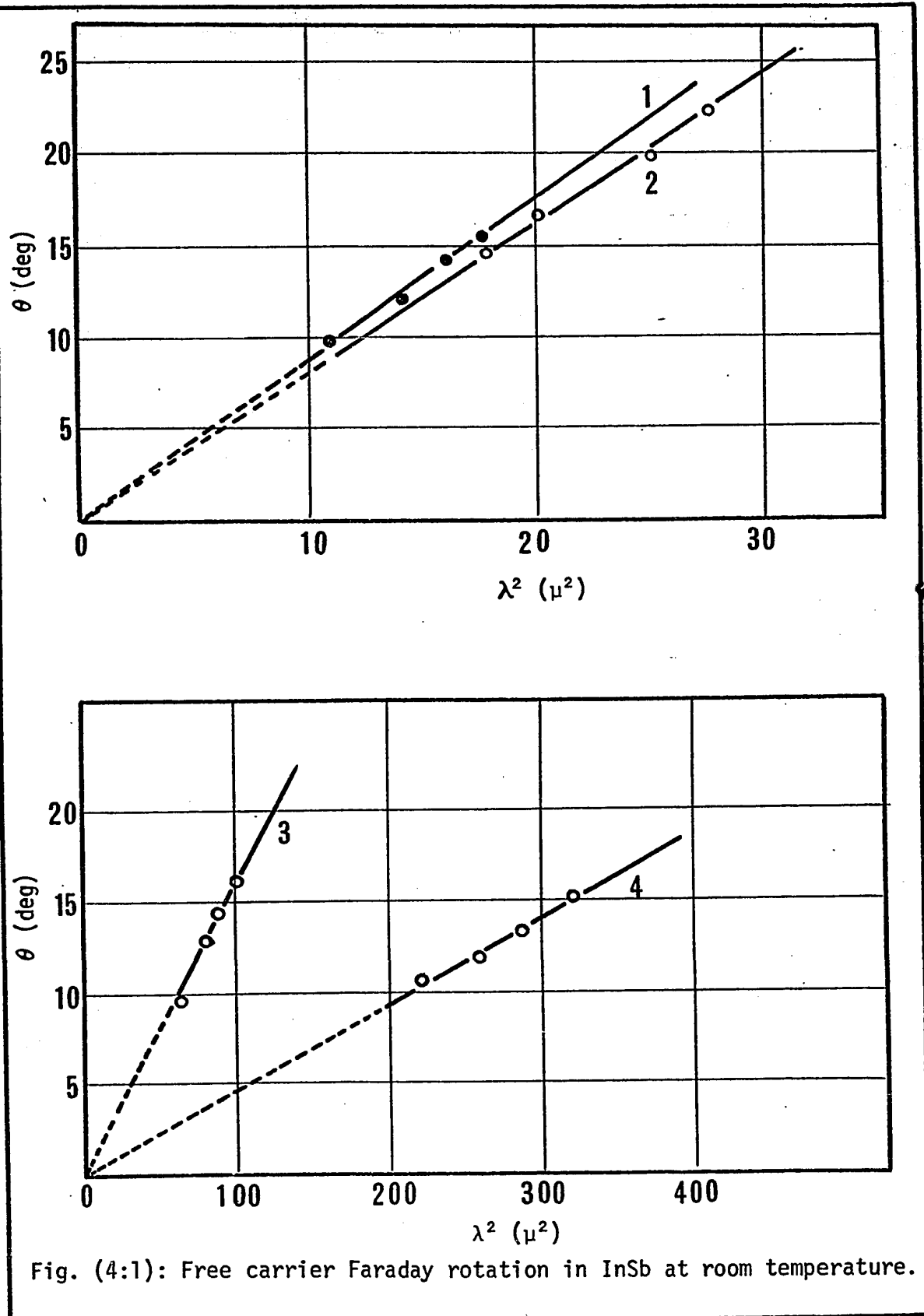
a) InSb

Four n-type polycrystalline specimen were prepared for the optical experiments. The different doping levels were obtained by adding amounts of tellurium to commercial polycrystalline InSb (n-type $\sim 10^{16}/\text{cm}^3$). The mixtures were melted under vacuum in a sealed quartz capsule and annealed for a few days.

The results of the Faraday rotation measurements are shown in figures (4: 1(a)) and (4: 1(b)). Other experimental data is listed in Table 4B.

The carrier concentration values for specimens 1 and 2 were obtained by magnetoresistance measurements made by Aubin⁷². For specimens 3 and 4 Hall effect measurements were made in the standard way without any variation of the magnetic field. A Hall current of 100ma and a Hall field of 0.73 w/m^2 were used.

In this table and following tables "Field" refers to the field used in the Faraday rotation measurements and "Slope" refers to the resultant slope of the rotation as the square of the wavelength.



Specimen number	Thickness (microns)	Carrier concentration ($\times 10^{16}/\text{cm}^3$)	Field (w/m^2)	Slope ($\times 10^{10} \text{deg}/\text{m}^2$)
1	244	774	0.711	86.0
2	224	307	0.711	80.0
3	208	15.4	0.700	15.8
4	212	3.83	0.700	4.62

T A B L E 4B

In table 4C the origin of the specimen and the different codings are shown

Specimen number	Source	Source's code	Other code
1	Aubin	S3	
2	Aubin	S13	
3	E.V.T.	1	1
4	E.V.T.	2	2

T A B L E 4C

In the column headed "OTHER CODE", the numbers are those given to these specimens in reference 80.

Thermoelectric power measurements were made on specimen #4. In order to investigate the effect of mica thickness on the value of α , the thermoelectric power coefficient, measurements were made on specimen #4 using four pieces of mica of thickness 32, 48, 64 and 80 microns. The results are shown in figure (4; 2). The extrapolated value at zero thickness is taken from the value quoted for a InSb specimen, of similar carrier concentration by Russian workers. If this reported value is taken to be correct it is seen that the thermoelectric power coefficient obtained by the method described in Chapter 3 can be expected to be about 5% too low when a single 32 μ sheet of mica is used as the electrical insulation. This thickness of mica was used in all the thermal measurements quoted here.

(b) GaAs

Two n-type single crystals of GaAs were obtained from Aubin and room temperature Faraday rotation measurements were made on these specimen. The results are shown in figure (4:3).

Values for the carrier concentration are shown in tables 4D. These values are found from room temperature magnetoresistance and Hall effect measurements made by Aubin⁷²

Specimen number	Thickness (microns)	Carrier concentration ($\times 10^{16}/\text{cm}^3$)	Field (w/m^2)	Slope ($\times 10^{10} \text{ deg/m}^2$)
5	513	395	0.702	101
6	578	83.2	0.702	31.8

T A B L E 4D

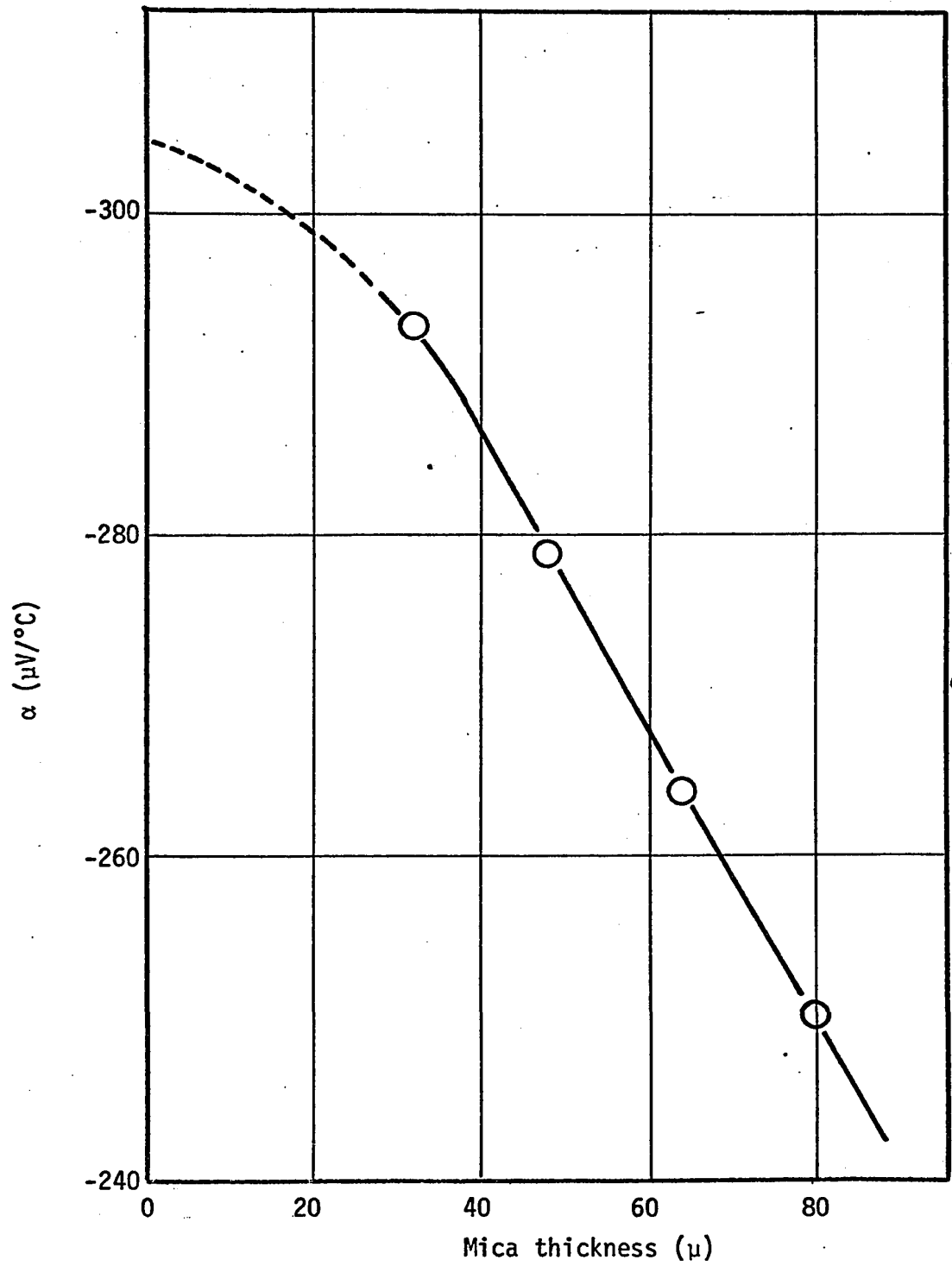


Fig. (4:2): Thermoelectric power vs mica thickness for specimen #4.

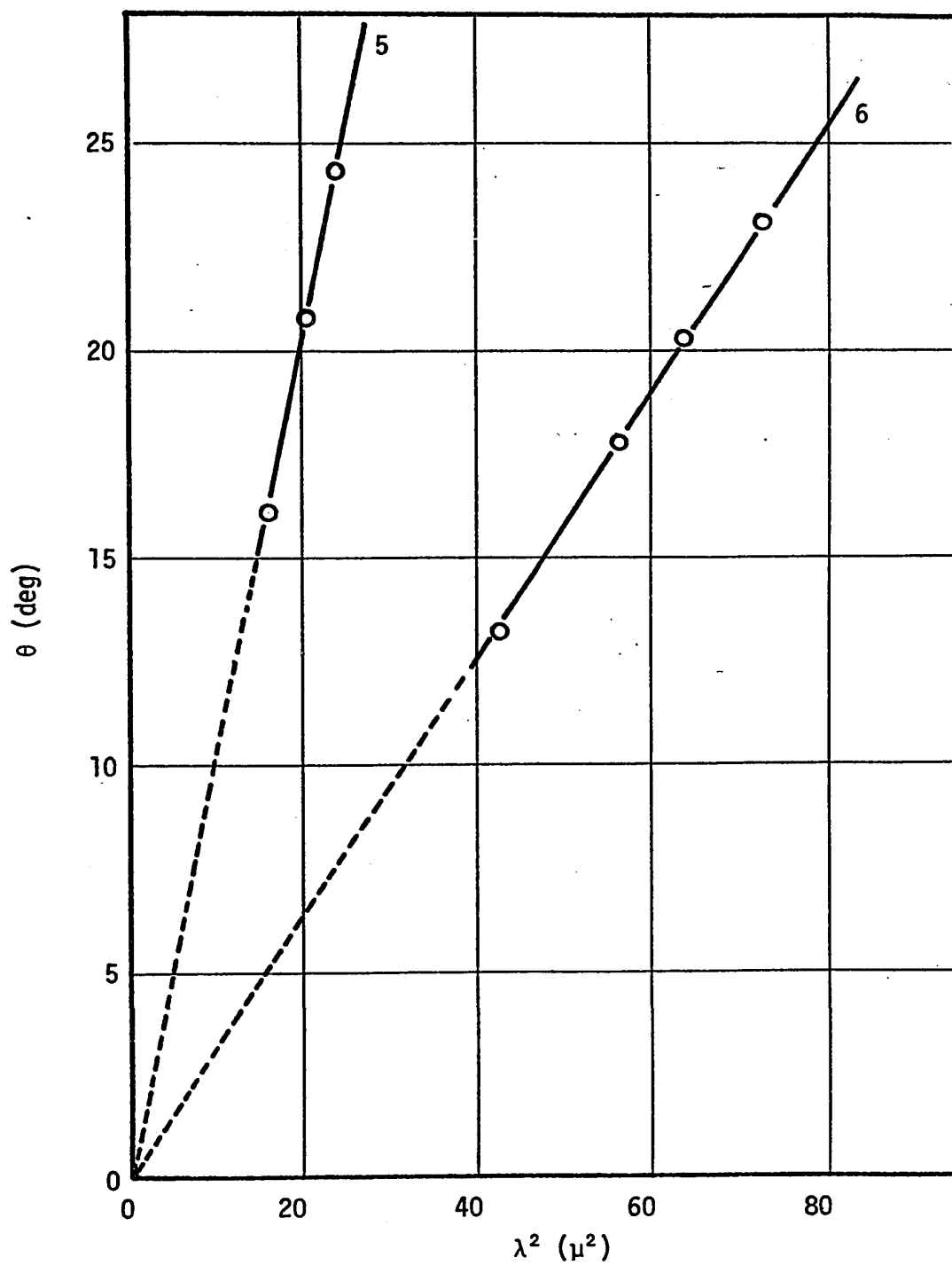


Fig. (4:3): Free carrier Faraday rotation in GaAs at room temperature.

c) GaSb

Four n-type tellurium doped GaSb single crystals were obtained from Harland^{74,75}. Magnetoresistance and Hall measurements as a function of temperature had been made on the specimens. Owing to the complexity of the band structure of GaSb, which will be expounded upon later, the value of the carrier concentration could not be obtained directly from the electrical measurements. These measurements yield values for $\frac{N_i}{r_i F_i}$ which are carrier concentrations factors for the *i*th conduction band minima. These factors have been described in Chapter 3.

Combining these experiments with room temperature Faraday rotation measurements permits a better analysis of this data. The results of the Faraday rotation measurements are shown in figure (4:4). Here the rotation is plotted as a function of wavelength and not as a function of the square of the wavelength since here the complexity of the band structure requires one to take into account inter-conduction band transitions. This is further discussed in Chapter 5.

Table 4E shows the results of other measurements. The numbers in the "SOURCE CODE" column refer to the specimen numbers given in reference 74, 75 and 76.

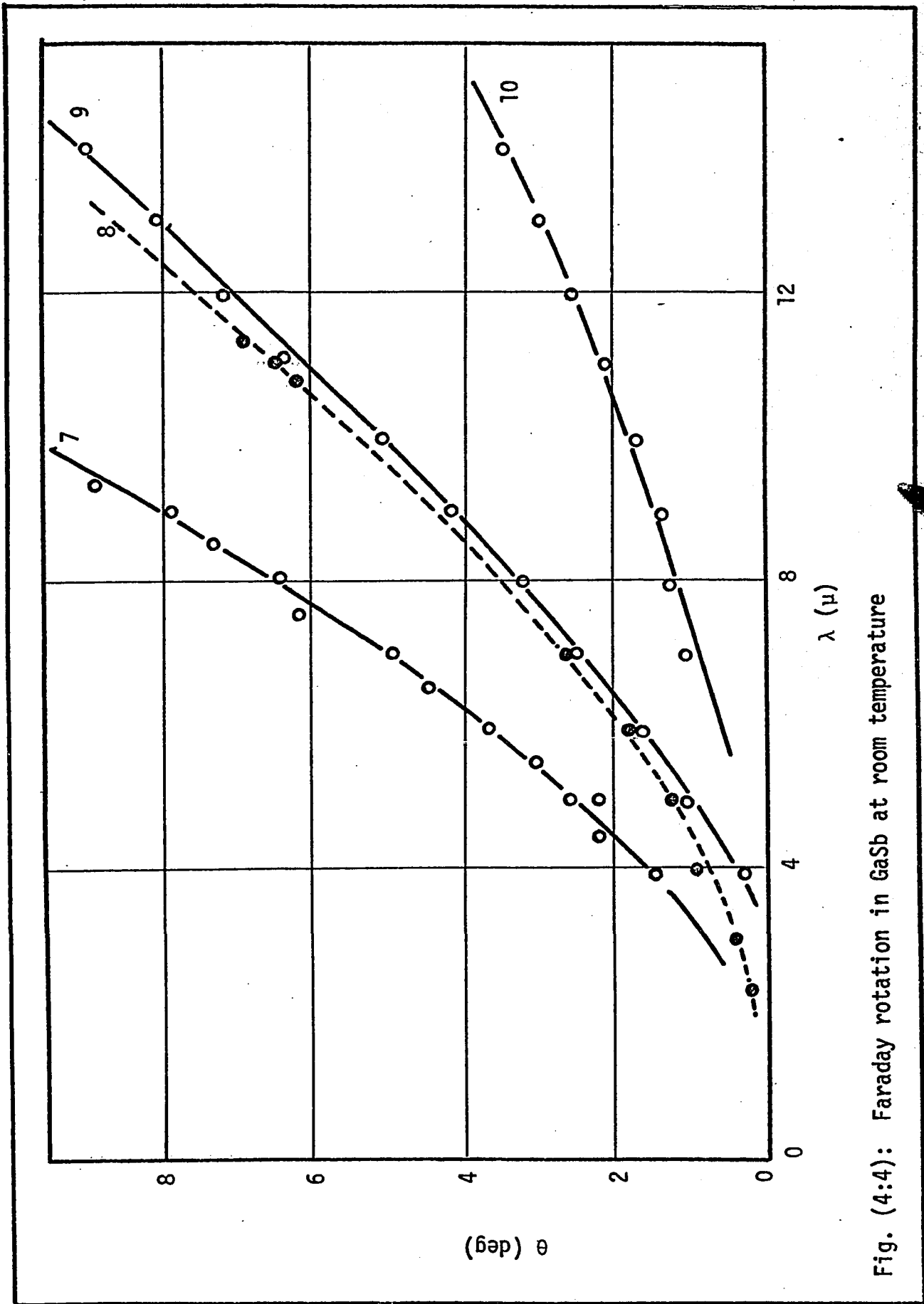


Fig. (4:4): Faraday rotation in GaSb at room temperature

Specimen number	Source code	Thickness (microns)	$N_o/r_o F_o$ ($\times 10^{16}/\text{cm}^3$)	$N_i/r_i F_i$ ($\times 10^{16}/\text{cm}^3$)	Faraday field w/m^2
7	6	119	58.05	251.3	0.61
8	8	140	28.71	110.1	0.61
9	10	190	16.39	47.63	0.73
10	9	150	7.937	20.86	0.70

T A B L E 4E

Some rough measurements of optical absorption indicated that the free carrier absorption was high and hence the effects of multiple internal reflections need not be considered here.

d) InAs

There is some difficulty involved in the preparation of differently doped InAs specimen. The specimens which were prepared by the author had a number of pinholes. These specimens were thus not suitable for either the electrical or optical measurements. This problem has been overcome and Kwan^{77,78} has performed a full analysis of InAs. A centrifuge method was used and this seems to produce good optical and electrical specimen. A complete Faraday rotation analysis will be performed by R. Senechal⁷⁹.

One InAs specimen was obtained from the stock of commercial InAs. Faraday rotation, Hall effect and thermoelectric power measurements were made on this specimen. In the Hall experiment the magnetic field was

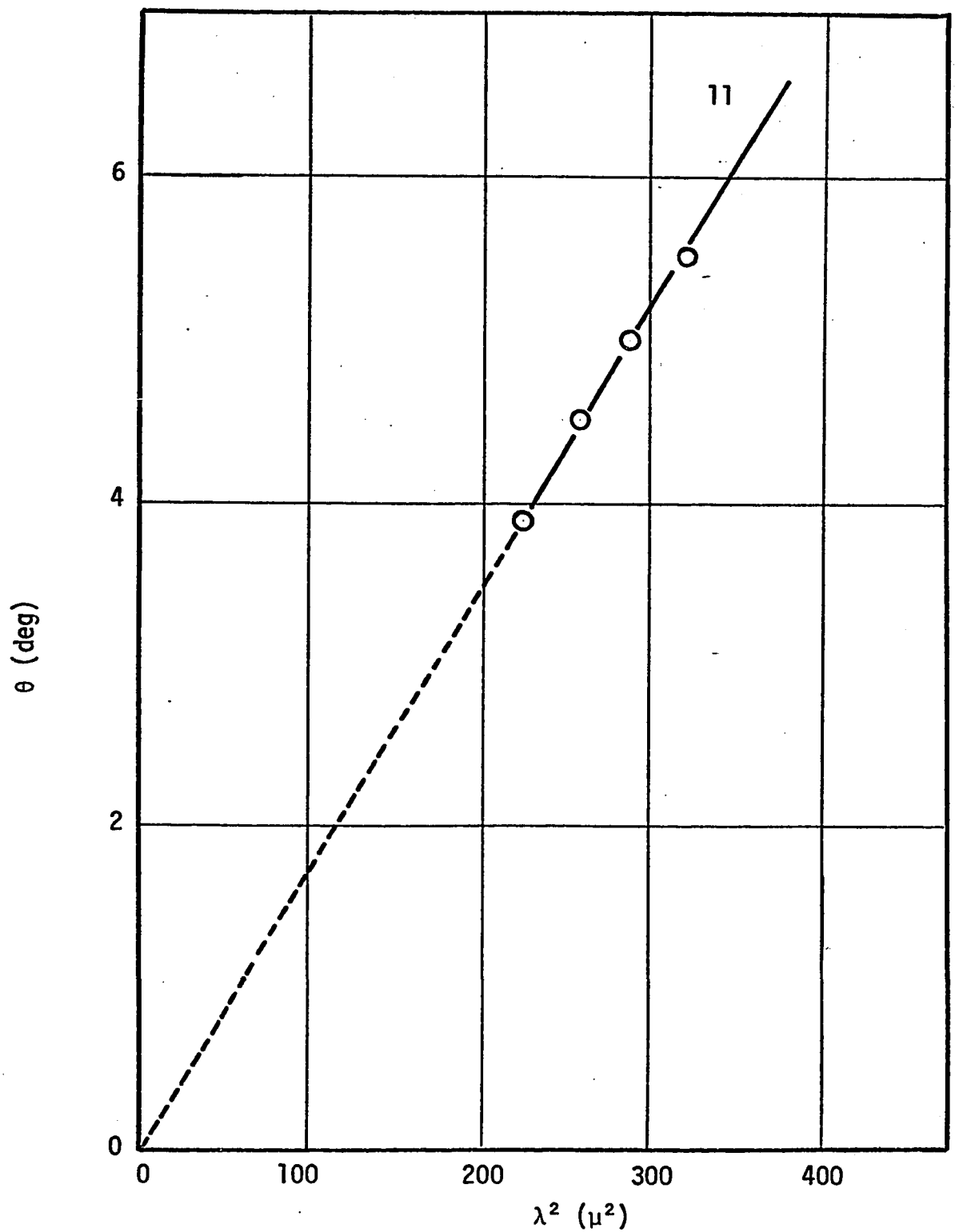


Fig. (4:5): Free carrier Faraday rotation in InAs at room temperature

0.73 w/m² and the current was 100 mA. The results of these measurements are shown in fig. [4:5] and Table 4F. The "OTHER CODE" refers to the number given to this specimen in reference 80

Specimen number	Other code	Thickness (microns)	Carrier concentration (x10 ¹⁶ /cm ³)	Field (w/m ²)	Slope (x10 ¹⁰ deg/m ²)	α (μ V/°C)
11	19	164	3.37	0.70	1.73	-338

T A B L E 4F

iii) Measurements on the Alloys:

a) $\text{InSb}_{1-x}\text{As}_x$

All the material used in this work was prepared by Coderre¹⁸. These specimen were found to be fairly homogeneous and X-ray powder photographs enabled the measurement of the lattice parameter to between 1% and 2%. The composition was then found by using previously published data of lattice parameter vs. composition²⁸. For convenience this curve is reproduced in Fig. (4:6). The composition was found using the solid curve rather than the dotted "Vegard's Law" straight line. Any uncertainty in the composition is thus generated by uncertainties in this curve.

Rough optical absorption measurements indicated firstly, that these specimen could not be considered to be degenerate since no Burstein shift was noticed⁴⁸. Secondly since the absorption was high the effects of multiple internal reflections were neglected in the analysis of the Faraday rotation data.

The measurement of free carrier Faraday rotation was made using both the "old" and the "new" methods. Table 4A indicates which method was used on each specimen. In order to check the "new" and faster technique both methods were used on specimen 22. The results, shown in figure (4:10) show that either method is satisfactory and will yield the same results. The results of the magneto-optical measurements are shown in Figures (4:7) to (4:9).

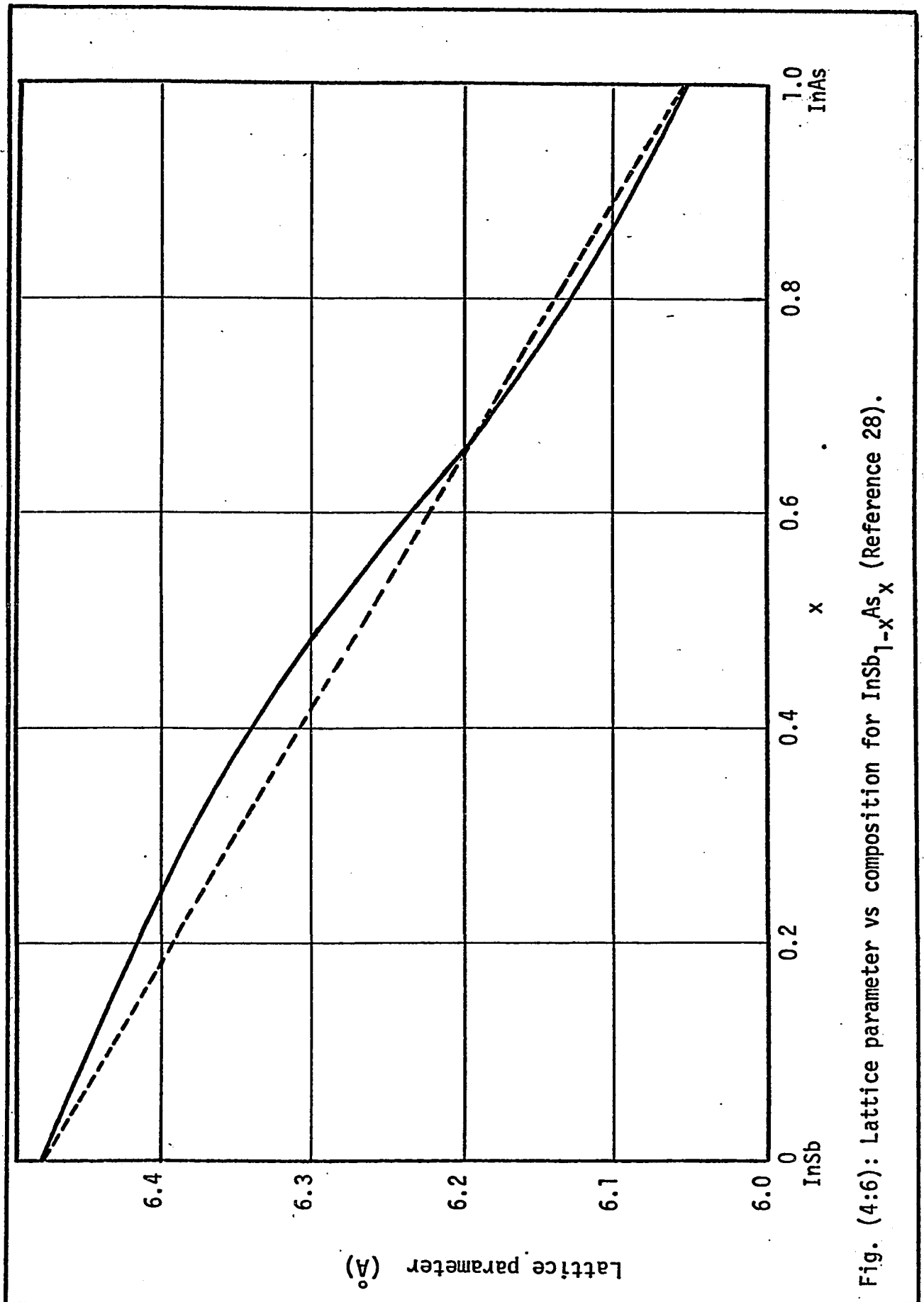


Fig. (4:6): Lattice parameter vs composition for $\text{InSb}_{1-x}\text{As}_x$ (Reference 28).

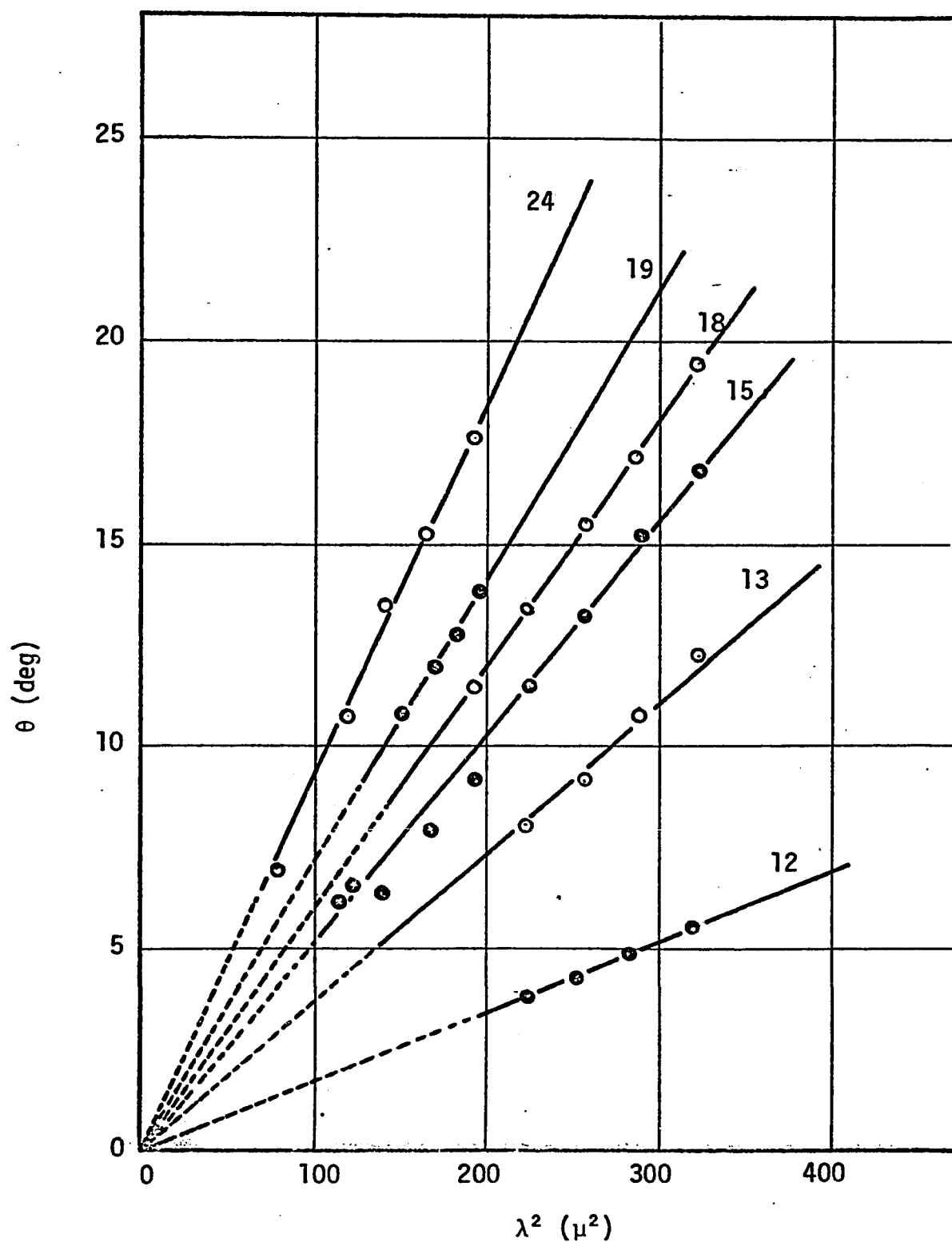


Fig. (4:7): Free carrier Faraday rotation in $\text{InSb}_{1-x}\text{As}_x$ at room temperature.

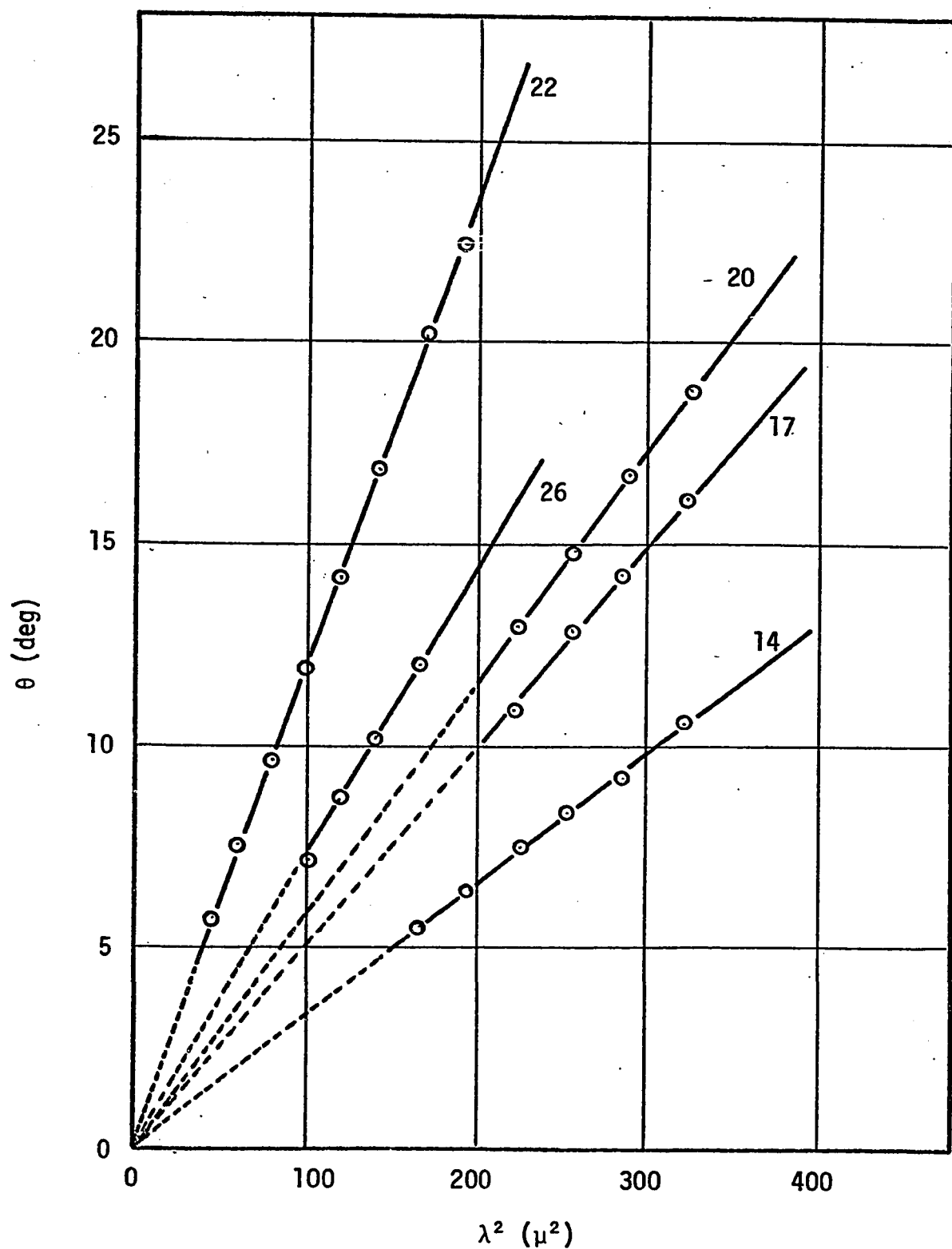


Fig. (4:8): Free carrier Faraday rotation in $\text{InSb}_{1-x}\text{As}_x$ at room temperature.

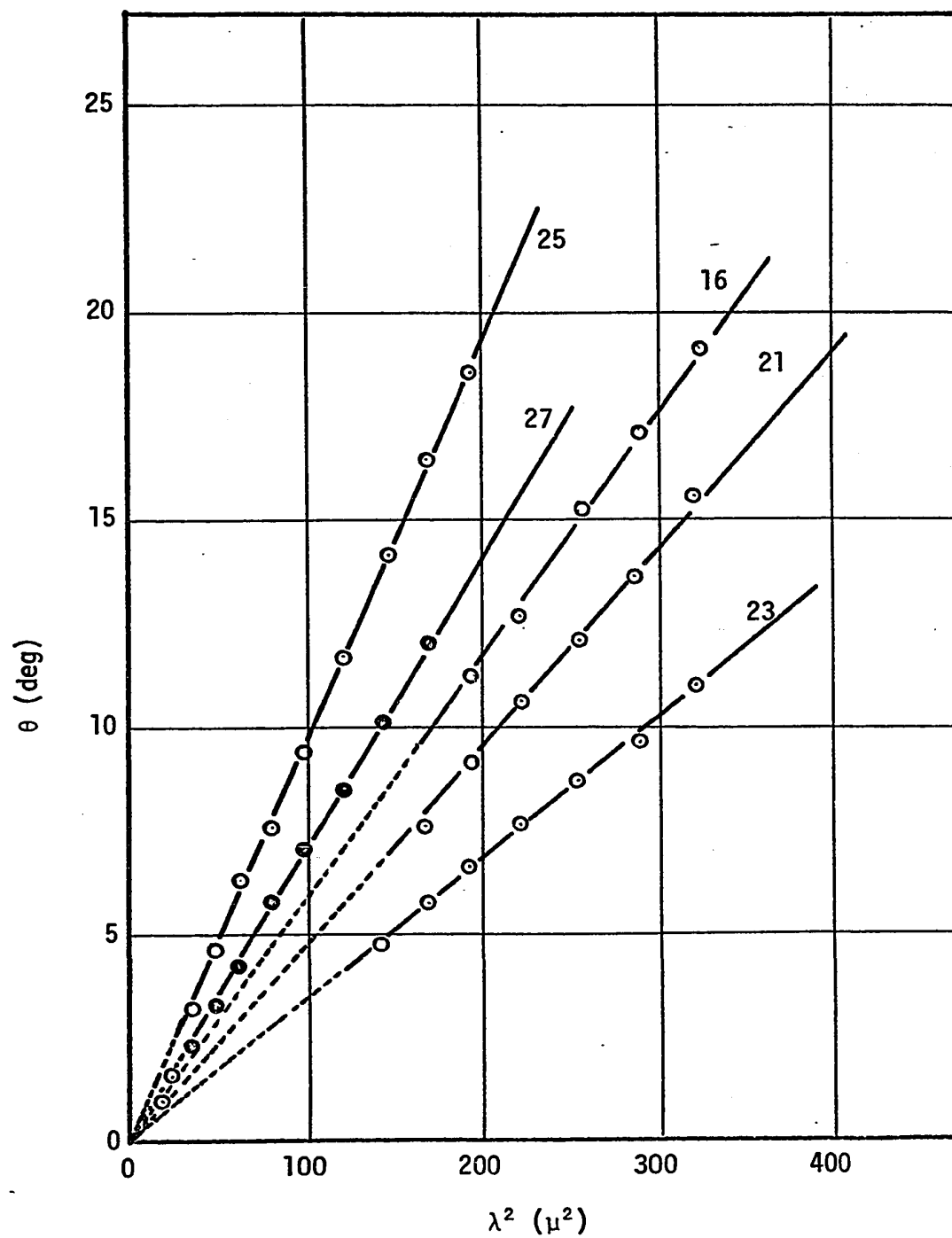


Fig. (4:9): Free carrier Faraday rotation in $\text{InSb}_{1-x}\text{As}_x$ at room temperature.

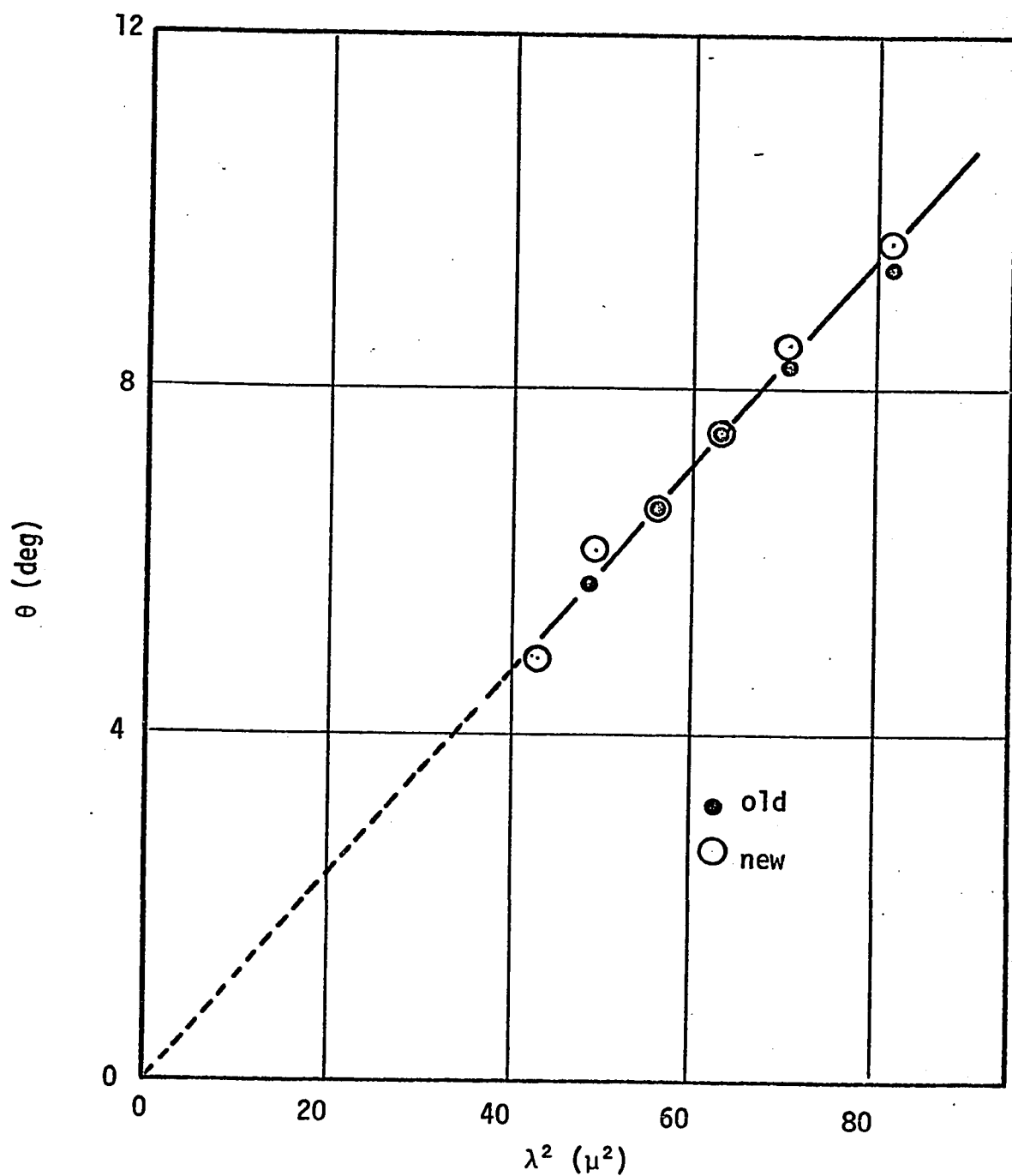


Fig. (4:10): Rotation in specimen #22 using "old" and "new" methods.

Hall effect measurements were made using the high field technique described in Chapter 3. Fig. (4:11) shows some typical results of these measurements. In some cases saturation of the Hall coefficient was not reached and for these the value at the largest attainable field was taken as the Hall coefficient at infinity.

Table 4G shows the results of the Hall effect and Faraday rotation measurements and in Table 4H the results of the X-ray and thermoelectric power measurements on some of the samples are shown. Table 4I indicates some other numbers which had been used to code these specimen. Here "OTHER CODE" refers to numbers from reference 80

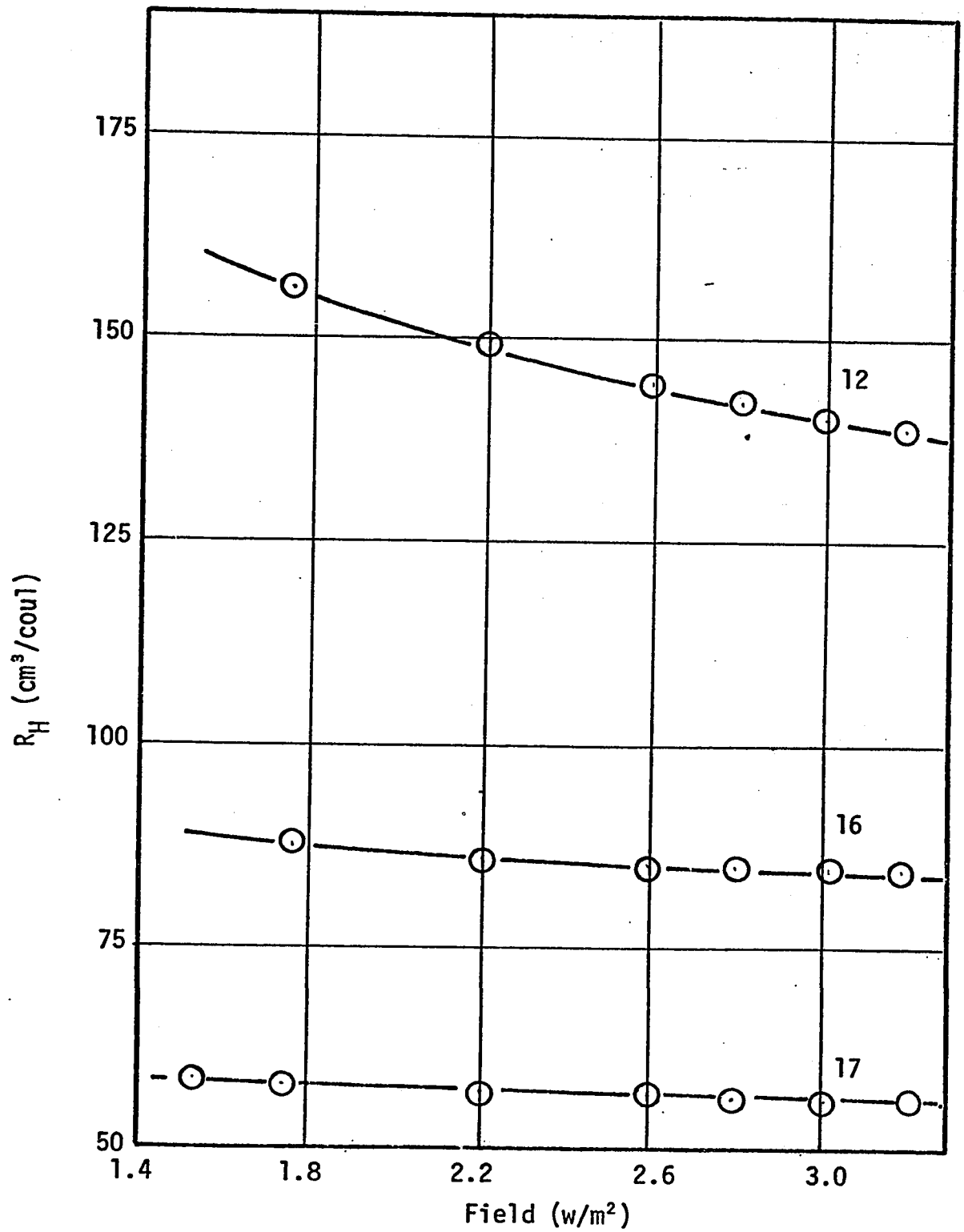


Fig. (4:11): Hall coefficient variation with magnetic field in $\text{InSb}_{1-x}\text{As}_x$.

Specimen number	Thickness (microns)	Carrier concentration ($\times 10^{16}/\text{cm}^3$)	Field (w/m^2)	Slope ($\times 10^{10} \text{deg}/\text{m}^2$)
12	67	4.66	0.700	1.69
13	109	5.71	0.700	3.78
14	83	5.76	0.700	3.28
15	103	8.64	0.700	5.17
16	126	7.41	0.700	5.89
17	90	11.3	0.700	4.98
18	105	8.38	0.700	6.02
19	129	9.99	0.700	6.97
20	131	8.71	0.700	5.77
21	97	8.56	0.700	4.73
22	152	11.7	0.725	11.6
23	103	8.48	0.700	4.4
24	97	20.8	0.700	9.13
25	182	13.9	0.700	9.72
26	109	18.9	0.725	7.11
27	235	7.72	0.725	6.98

T A B L E 4G

Specimen number	Lattice parameter (Å)	Composition x	α ($\mu\text{V}/^\circ\text{C}$)
12	6.454	0.09	-277
13	6.443	0.15	-202
14	6.421	0.19	-226
15	6.400	0.25	-169
16	6.365	0.34	
17	6.337	0.40	-191
18	6.319	0.44	
19	6.276	0.535	
20	6.216	0.635	
21	6.186	0.68	
22	6.168	0.71	-177
23	6.141	0.775	
24	6.100	0.87	
25	6.085	0.91	
26	6.078	0.935	-219
27	6.070	0.960	-273

T A B L E 4H

Specimen number	Laboratory code	Other code
12	TZ-C-3 (8.37)	3
13	TZ-C-1 (3.68)	4
14	TZ-C-1 (3.20)	5
15	TZ-C-1 (3.43)	6
16	TF-C-1 (3.70)	7
17	TZ-C-3 (7.60)	8
18	TF-C-1 (3.48)	9
19	TF-C-1 (3.25)	10
20	TF-C-1 (3.07)	11
21	TF-C-1 (2.95)	12
22	TZ-C-1 (3.25)	13
23	TF-C-1 (2.46)	14
24	TZ-C-5(13.5)	15
25	TZ-C-1 (2.70)	16
26	TZ-C-1 (2.00)	17
27	TZ-C-1 (0.81)	18

T A B L E 4I

b) $\text{In}_{1-x}\text{Ga}_x\text{Sb}$

The measurements on specimens of this system were made on samples obtained from a single ingot prepared by the author using the directional freeze technique mentioned in Chapter 3 and more fully described in reference 18. X-ray powder photographs showed these specimens to be of good homogeneity. The lattice parameter could in these cases be found to better than 1%. The composition was then found from previously published data of the lattice parameter as a function of the composition²⁶ and these results are reproduced in figure (4:12).

Since the doping level of this ingot was fairly high the Hall measurements in increasing magnetic field showed a saturation of the Hall coefficient in increasing magnetic field for all specimen. The Hall coefficient values from 2.0 to 3.2 w/m^2 showed a variation only in the fourth figure and hence the carrier concentration was calculated from the average of the values at the above fields.

At these electron concentrations (generally greater than $5 \times 10^{17}/\text{cm}^3$) absorption of infrared radiation is high even at wavelengths much longer than the fundamental gap. This is due to free carrier absorption. The absorption curves for some specimen are shown in figure (4:13). Here the absorption is plotted against the square of the radiation wavelength to show the linear behaviour of the free carrier effect. In these curves I_0 is the radiant intensity without the specimen and I is the radiant intensity after traversing the specimen. These high absorption levels

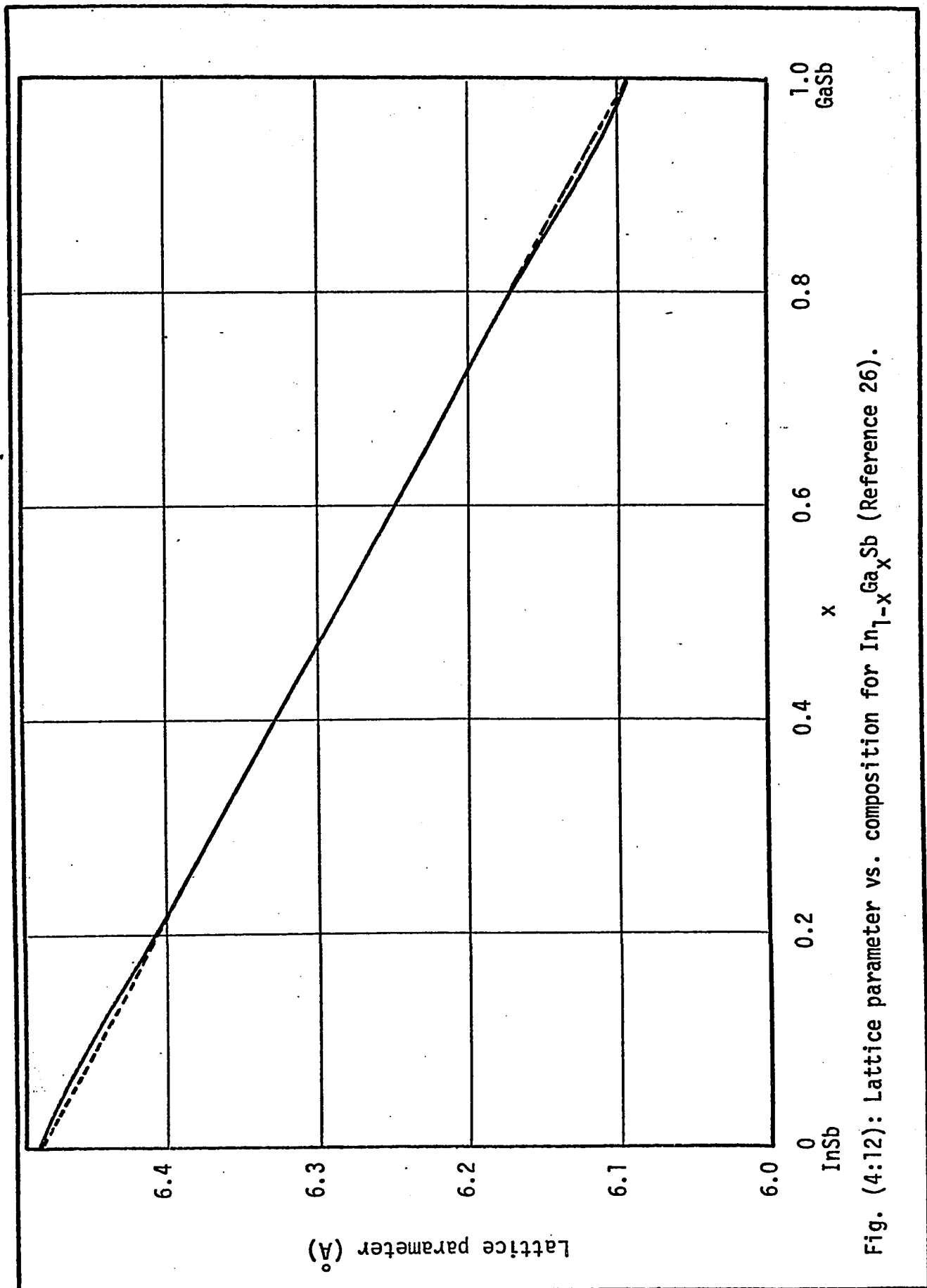


Fig. (4:12): Lattice parameter vs. composition for $\text{In}_{1-x}\text{Ga}_x\text{Sb}$ (Reference 26).

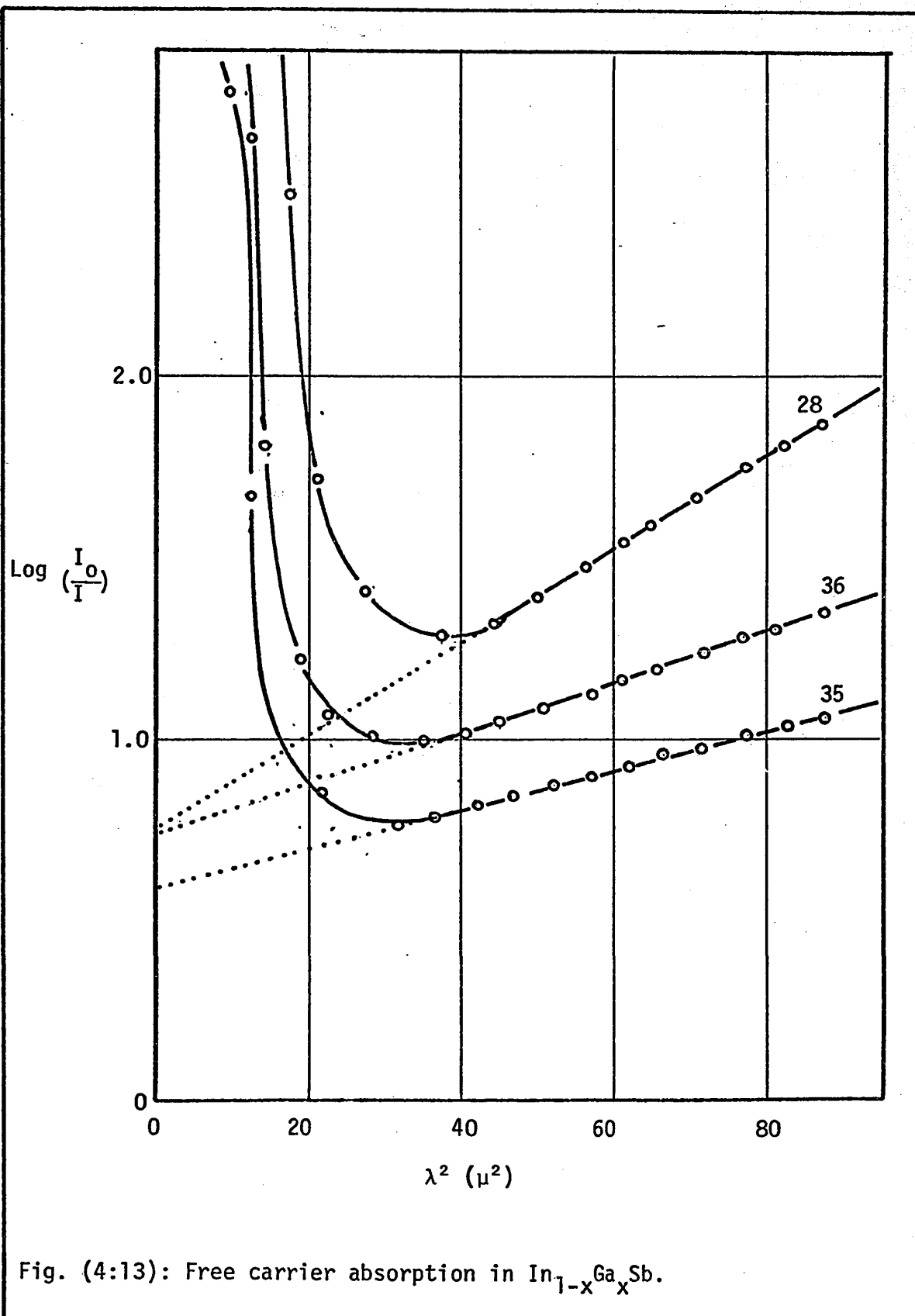


Fig. (4:13): Free carrier absorption in $\text{In}_{1-x}\text{Ga}_x\text{Sb}$.

again permit one to neglect the effects of multiple internal reflections in the analysis of the Faraday rotation data.

Since the results of these measurements were to be combined with magneto thermoelectric power data of Aubin^{72,81} no thermal measurements were made.

The Faraday rotation results are shown in figures (4:14) to (4:16) and the data from these and other measurements are tabulated in Table 4J.

The results of the X-ray analysis and the optical absorption curves are shown in Table 4K

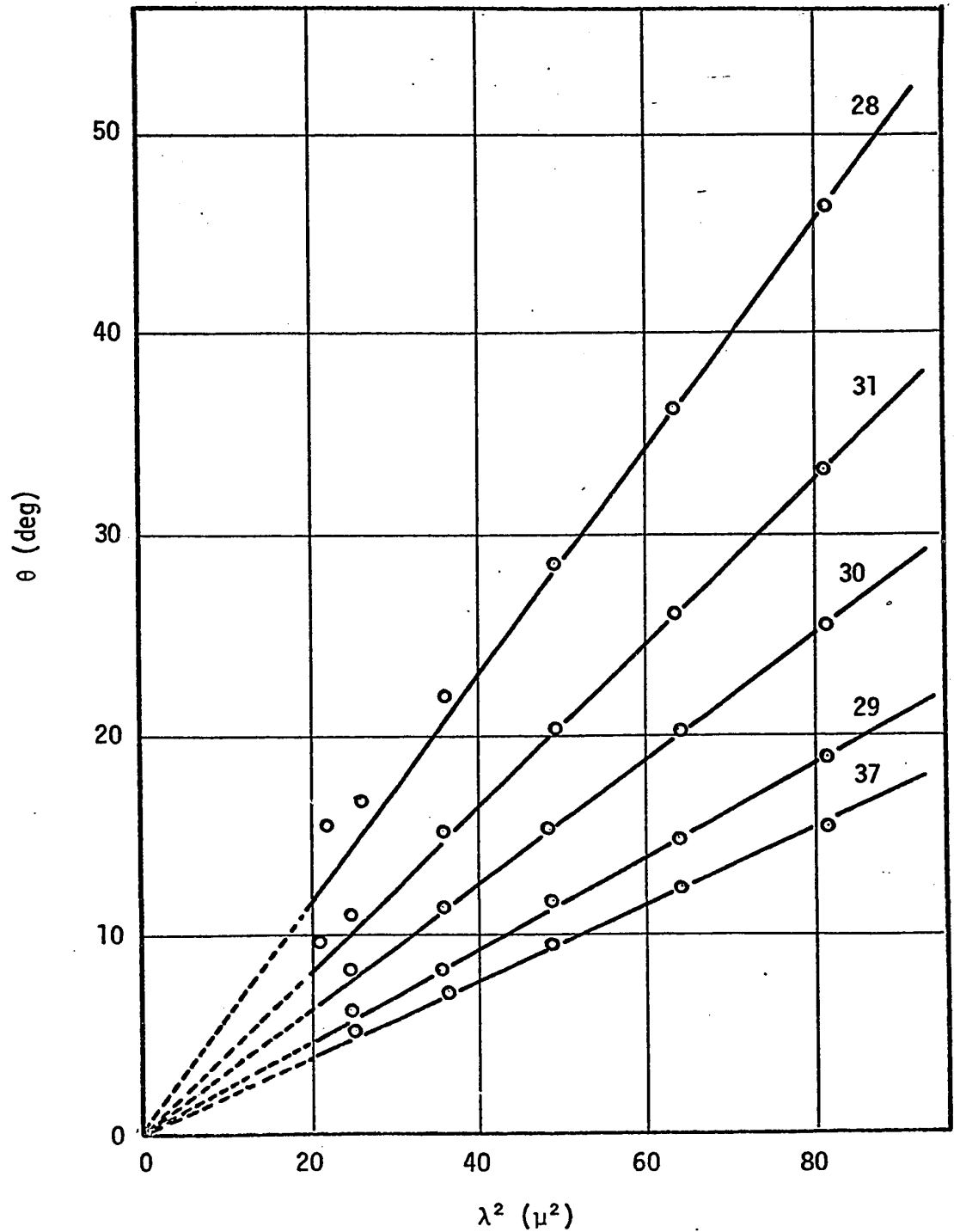


Fig. (4:14): Faraday rotation in $\text{In}_{1-x}\text{Ga}_x\text{Sb}$ at room temperature.

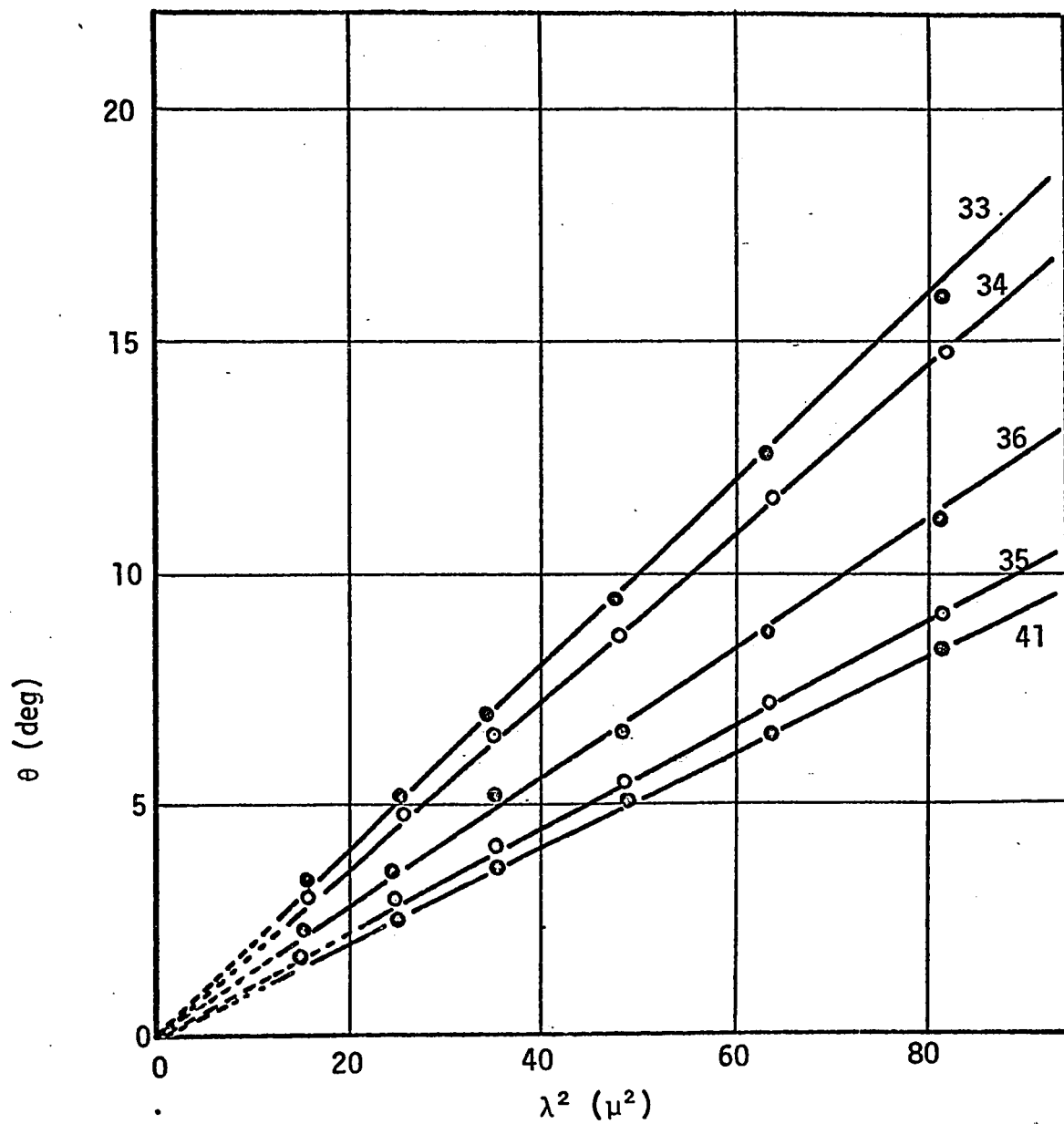


Fig. (4:15): Faraday rotation in $\text{In}_{1-x}\text{Ga}_x\text{Sb}$ at room temperature.

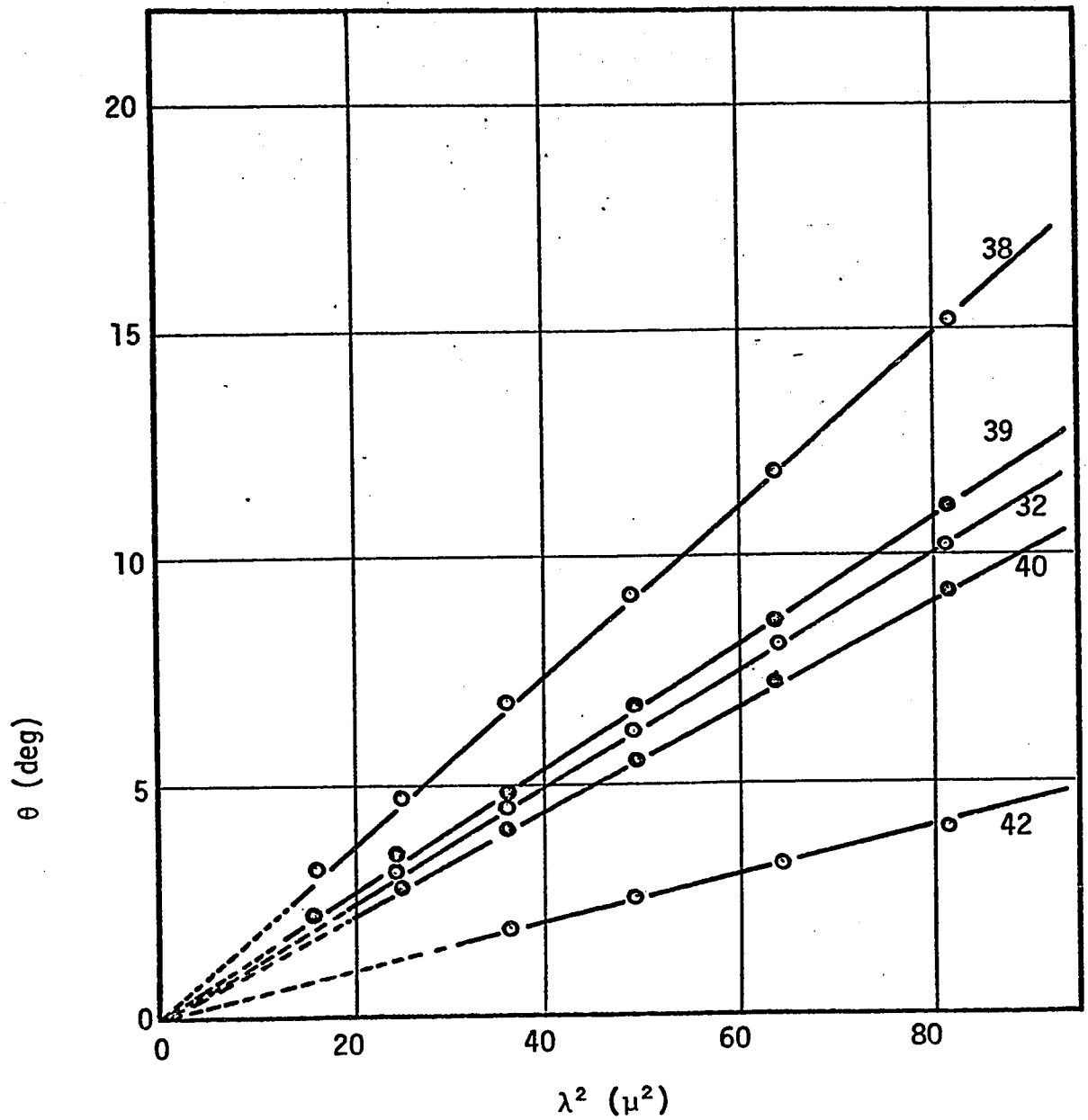


Fig. (4:16): Faraday rotation in $\text{In}_{1-x}\text{Ga}_x\text{Sb}$ at room temperature.

Specimen number	Thickness (microns)	Carrier concentration ($\times 10^{16}/\text{cm}^3$)	Field (w/m^2)	Slope ($\times 10^{10} \text{ deg}/\text{m}^2$)
28	226	109	0.728	57.2
29	87	128	0.702	23.3
30	179	90.0	0.702	31.6
31	235	73.8	0.728	42.0
32	104	69.6	0.702	12.5
33	114	83.3	0.702	19.4
34	150	68.0	0.702	18.7
35	73	72.7	0.702	11.0
36	130	58.2	0.702	13.7
37	177	56.4	0.728	19.3
38	171	53.9	0.702	18.9
39	131	55.4	0.702	13.4
40	129	54.6	0.702	11.6
41	140	40.3	0.702	10.4
42	130	23.3	0.702	4.87

T A B L E 4J

Specimen number	Lattice parameter (Å)	Composition x	Absorption Slope ($\times 10^{10}/\text{m}^2$)	Laboratory code
28	6.425	0.160	1.24	DF-A-8 (11.8)
29	6.411	0.195	0.758	" (9.8)
30	6.373	0.290	0.448	" (8.2)
31	6.349	0.350	0.890	" (7.1)
32	6.331	0.400	0.636	" (6.43)
33	6.331	0.400	0.870	" (6.23)
34	6.303	0.470		" (5.03)
35	6.300	0.480	0.480	" (5.43)
36	6.293	0.500	0.718	" (5.23)
37	6.290	0.510	0.640	" (4.73)
38	6.282	0.530	0.668	" (5.13)
39	6.269	0.560		" (3.93)
40	6.253	0.600		" (4.13)
41	6.241	0.630		" (3.53)
42	6.200	0.730		" (1.67)

T A B L E 4K

CHAPTER 5

A N A L Y S I S O F E X P E R I M E N T A L D A T A

Introduction:

The analysis of the Faraday rotation data was carried out in a slightly different way for some specimens than the rest. This was due, as will be seen, to the degree of degeneracy of these specimens or to the complexity of the band structure. For this reason an outline of the rules to be followed in analysing free carrier Faraday rotation data, will be given first. A more detailed account of the analysis will then be given when each set of measurements will be analysed in a specific way. It must be pointed out here that in general the purpose of this work was to calculate the value of the bottom of the band effective mass, m_{00}^* , and this was done in the case of InSb (specimens 3 and 4), InAs and the two alloy systems. For the case of GaSb, however a value for m_{00}^* was assumed in the hope that more information about the $\langle 111 \rangle$ conduction band could be found. In all cases a Kane model was chosen to represent the (000) conduction band. In the case of InSb some estimate of the suitability of this choice could be given by comparing the results obtained from low degenerate specimens with those of higher degeneracy.

ii) Free Carrier Faraday Rotation:

From equation [2:4] it can be seen that the slope of the θ vs λ^2 plots can yield a value for the Faraday or cyclotron effective mass. This is given by the equation

$$S_1 = (1.509 \times 10^{-11}) \frac{B t n_i}{\eta (m_i^*/m)^2} \dots\dots\dots [5:1]$$

where S_1 is the slope of these lines. There are however four conditions which are inherent in equation [5:1] and these must be considered before [5:1] is to be used.

a) Firstly in order to find a value for the effective mass from [5:1] the refractive index, η , must be known. The value of η , however, is a function of the degree of doping of the specimen. For low doped specimen the free carrier absorption is low and the contribution to η due to this effect is negligible. In this case in the wavelength range under consideration here, 4 - 20 microns, η can be considered to be wavelength independent and is given by

$$\eta = (\epsilon_r)^{\frac{1}{2}} \dots\dots\dots [5:2]$$

where ϵ_r , as in equation [2:2] is the specific dielectric constant of the material in the absence of free carriers. Where required, values for ϵ_r are taken from reference 86.

At higher carrier concentrations, however, the free carrier absorption becomes appreciable and the refractive index for the wavelength range quoted above, changes with wavelength. The relation for this dependence is given by equation [2:3] which, in the absence of magnetic fields ($\omega_c = 0$ and m_{ic}^* is replaced by m_{iR}^*) and under the assumption that at these wavelengths $\omega\tau \gg 1$, becomes

$$\eta^2 = \epsilon_r - \frac{e^2}{4\pi^2 c^2 \epsilon_0} \left(\frac{n_i}{m_{iR}^*} \right) \lambda^2 \dots \dots \dots [5:3]$$

Here m_{iR}^* is the reflectivity effective mass but, as has been mentioned in Chapter 1, for single bands with associated spherical energy surfaces $m_{oR}^* = m_{oc}^*$. In this case equation [5:1] and [5:3] can be solved for m_{oc}^* using a cyclical continuous approximation method.

b) The second consideration which must be taken into account is the meaning of the effective mass value obtained at different levels of degeneracy. For fully degenerate specimen ($E_{Fi} > 4kT$) the effective mass value obtained by using [5:1] and [5:3] as indicated above, can be interpreted as the cyclotron mass evaluated at the Fermi level as in [2:5]. This of course implies the same conditions of a single band and spherical energy surfaces. Thus here

$$\frac{1}{m_{oc}^*} = \frac{1}{\hbar^2} \frac{1}{k_{Fo}} \frac{dE}{dk} \Big|_{Fo} \dots \dots \dots [5:4]$$

where $k_{F0}^3 = 3\pi^2 n_0$ [5:5]

How [5:4] and [5:5] are used will be shown in section (iii) of this chapter.

c) When the specimens cannot be considered to be fully degenerate the effective mass value obtained from [5:1] and [5:2] or from [5:1] and [5:3] must be interpreted as an average value over all the occupied states in the band but there is no way of telling which energy state will have this value. In these cases the only band parameter which can be found directly is the bottom of the band effective mass, m_{00}^* . If one assumes a Kane type dispersion law for the (000) conduction band then using equation [2:39] the slope of the θ vs λ^2 plots is given by

$$S_2 = \frac{60e^3 a^3 t B}{\pi^5 \hbar^4 c^3 \epsilon_0 n} \left(\frac{I_1}{kT} \right)$$

or $S_2 = D_1 \left(\frac{Bt}{n} \right) I_1$ [5:6]

where $D_1 = 45e^3 / 8\pi^6 \hbar^4 c^3 \epsilon_0 = 2.096 \times 10^{25}$ in rationalized MKS units. I_1 is given by [2:37]. Using [2:40] and [2:38] it can be shown that under the conditions of a single band with spherical energy surfaces.

$$\left(\frac{n_o}{m_o^* R/m}\right) = \left[\frac{n_o I_1}{16\pi^3 a^2}\right]^{\frac{1}{2}} \dots\dots\dots [5:7]$$

Replacing [5:7] into [5:3] yields

$$\eta^2 = \epsilon_r - \frac{e^2}{4\pi^2 c^2 \epsilon_o m} \left[\frac{n_o I_1}{16\pi^3 a^2}\right]^{\frac{1}{2}} \lambda^2 \dots\dots\dots [5:8]$$

Here then a cyclical continuous approximation technique using [5:6] and [5:8] will correct η for free carrier effects and yield the best value for I_1 . The way this is best accomplished is to find a starting value for I_1 from [5:6] using [5:2]. This value of I_1 is inserted into [5:8] and the value of η found at each wavelength is used to curve fit by a least squares method. The equation of Y vs λ^2 is given below

$$Y = \eta\theta = D_1 B t I_1 \lambda^2 \dots\dots\dots [5:9]$$

From this curve fit a new value of I_1 is obtained and recycled until two consecutive values for I_1 are the same.

Once the best value of I_1 has been obtained use is made of equation [2:37] and [2:38]. These two equations relate the experimental values of I_1 and n_o to the band structure. Equations [2:37] and [2:38] were therefore, numerically integrated using Simpson's rule with about 1000 divisions. The theoretically calculated values for I_1 and n_o were then

compared with the experimental values. There are, however, three unknowns, m_{00}^* , E_{F0} and E_0^* , in these two equations. Initially in order to obtain a solution various sets of values for m_{00}^* and E_{F0} were used for each value of E_0^* .

From the discussion in Chapter 3 section (iv) the expected range of E_0^* is between E_{00} and $E_0(T)$, the fundamental energy gap at absolute zero and the fundamental gap at temperature T . Therefore $E_0^* = E_0 + \delta E_0$ where $0 < \delta E_0 < (E_{00} - E_0)$.

In the trial solution of [2:37] and [2:38] it was found that the values of E_{F0} and m_{00}^* were insensitive to the value of δE_0 . In practice, a 50% variation in δE_0 caused a 6% change in m_{00}^* . In all cases, therefore, the value of δE_0 was arbitrarily taken as being $\frac{1}{2} (E_{00} - E_0)$. In this case $E_0^* = \frac{1}{2} (E_{00} + E_0)$ which physically implies that the effect of the dilation of the lattice is equal in magnitude to the effect of thermal vibrations in the decreasing of the energy gap with temperature. There is some reported evidence for this⁵⁸.

At these values for E_0^* solutions for [2:37] and [2:38] could be found by finding the sets of values for m_{00}^* and E_{F0} which would give the same theoretical value of I_1 as that measured and then independently finding the sets which would give the same theoretical value of n_0 as that measured. The resultant sets of solutions could then be plotted and the intersection of these curves gave the common solution. These will be

shown in later sections.

d) The fourth consideration to be made is the number of different conduction bands which could have occupied states. At most, in the case of the specimens considered here, only two bands need to be considered, the (000) band and the <111> band. It has been shown that for two conduction band processes the Faraday rotation is related to the radiation wavelength in the free carrier region by⁴²

$$\theta = \frac{45e^3 t B}{2\pi^3 m^2 c^3 \epsilon_0} \left[\frac{n_0}{(m_{0F}^*/m)^2} + \frac{n_1}{(m_{1F}^*/m)^2} \right] \frac{\lambda^2}{n(\lambda)} + \frac{AB}{\lambda^2} \dots\dots\dots [5:10]$$

where the first expression on the right hand side of the equation is due to free carrier effects only and the second term is the contribution due to inter-conduction band transitions. The refractive index in this case is written as⁴²

$$n^2 = \epsilon_r - \frac{e^2}{4\pi^2 c^2 \epsilon_0 m} \left[\frac{n_0}{(m_{0R}^*/m)} + \frac{n_1}{(m_{1R}^*/m)} \right] \lambda^2 \dots\dots\dots [5:11]$$

The relation between m_{iF}^* and m_{iR}^* is given in Chapter 1. More will be said about these equations in later sections.

iii) InSb

Since the specimens 1 and 2 were highly doped the Faraday rotation data were analysed using conditions (a), (b) and (d) mentioned previously. In the case of these specimens, however, the contribution to the rotation due to the $\langle 111 \rangle$ band is small because of the small effective mass values of the (000) electrons and hence condition (d) could be neglected. The results obtained using (a) and (b) were combined with the results of Smith, Moss and Taylor⁴⁹. These are tabulated in Table 5A. Here the results from reference 49 are listed as SMT.

Specimen number	n_0 ($\times 10^{22}/\text{m}^3$)	k_{F0} ($\times 10^7 \text{m}^{-1}$)	$\frac{m_{0c}^*}{m}$
1	774	61.2	0.0768
2	307	45.0	0.0505
SMT	64	22.7	0.029
SMT	20	18.1	0.022
SMT	2.9	9.5	0.0178
SMT	1.1	6.9	0.0165
SMT	0.26	4.2	0.0131
SMT	0.03	2.1	0.0130

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Figure (5: 1(a)) shows the variation of the slope $(\frac{dE}{dk}|_{F_0})$ with k_{F_0} obtained by using equation [5:4] and the results in Table 5A. Integrating this curve gives the variation of energy in k -space. This is shown in figure (5: 1(b)). Although this graph is not accurate in some regions it does give some idea as to the structure of the (000) band.

Specimens 3 and 4 were analysed using the technique described in (c) of the previous section. A print out of the computer program can be found in the appendix. Figure (5: 2) shows how a common solution can be obtained. The curves marked n_0 are those sets of $\frac{m_{00}^*}{m}$ and E_{F_0} which will yield the same value of n_0 calculated as that measured and similarly the curves marked I_1 are those sets of $\frac{m_{00}^*}{m}$ and E_{F_0} which yield the same calculated value of I_1 as that measured. The two values of $\frac{m_{00}^*}{m}$ obtained for each specimen agree to within 4%. The average of these values gives $(\frac{m_{00}^*}{m}) = 0.013$ for InSb at room temperature when a value of $E_0^* = \frac{1}{2} (0.24 + 0.18) = 0.21\text{eV}$ is used^{84, 85}. This value agrees with that obtained by Smith et.al.⁵⁰.

In order to illustrate the effect of uncertainties in δE_0 , an analysis was carried out on the results from specimen 3. This is shown in figure (5: 3). The importance of knowing δE_0 accurately is seen to be not too critical. The complete results of specimen 3 and 4 will be given later with the alloy results.

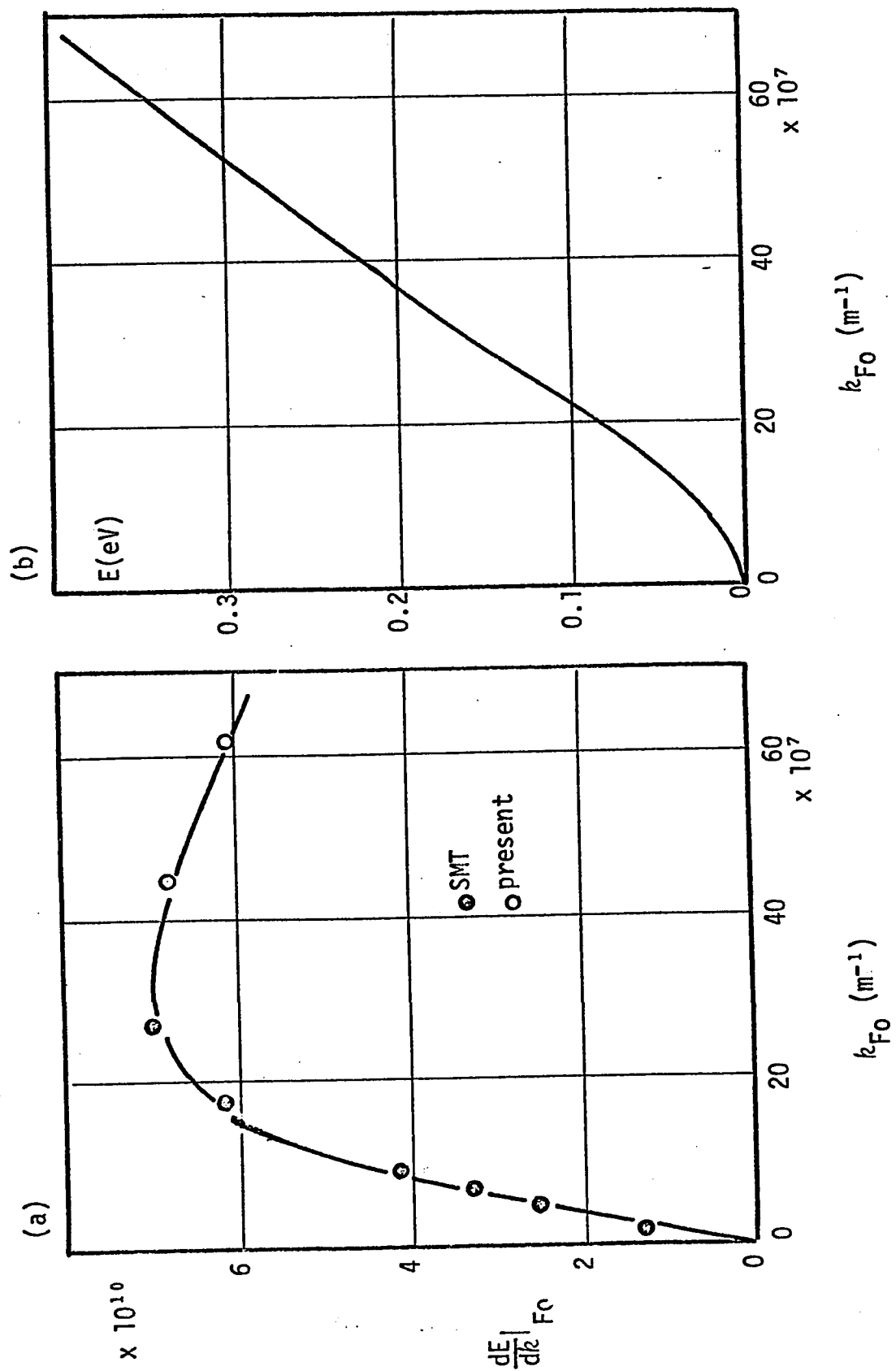


Fig. (5:1): Band structure of InSb from Faraday rotation data.

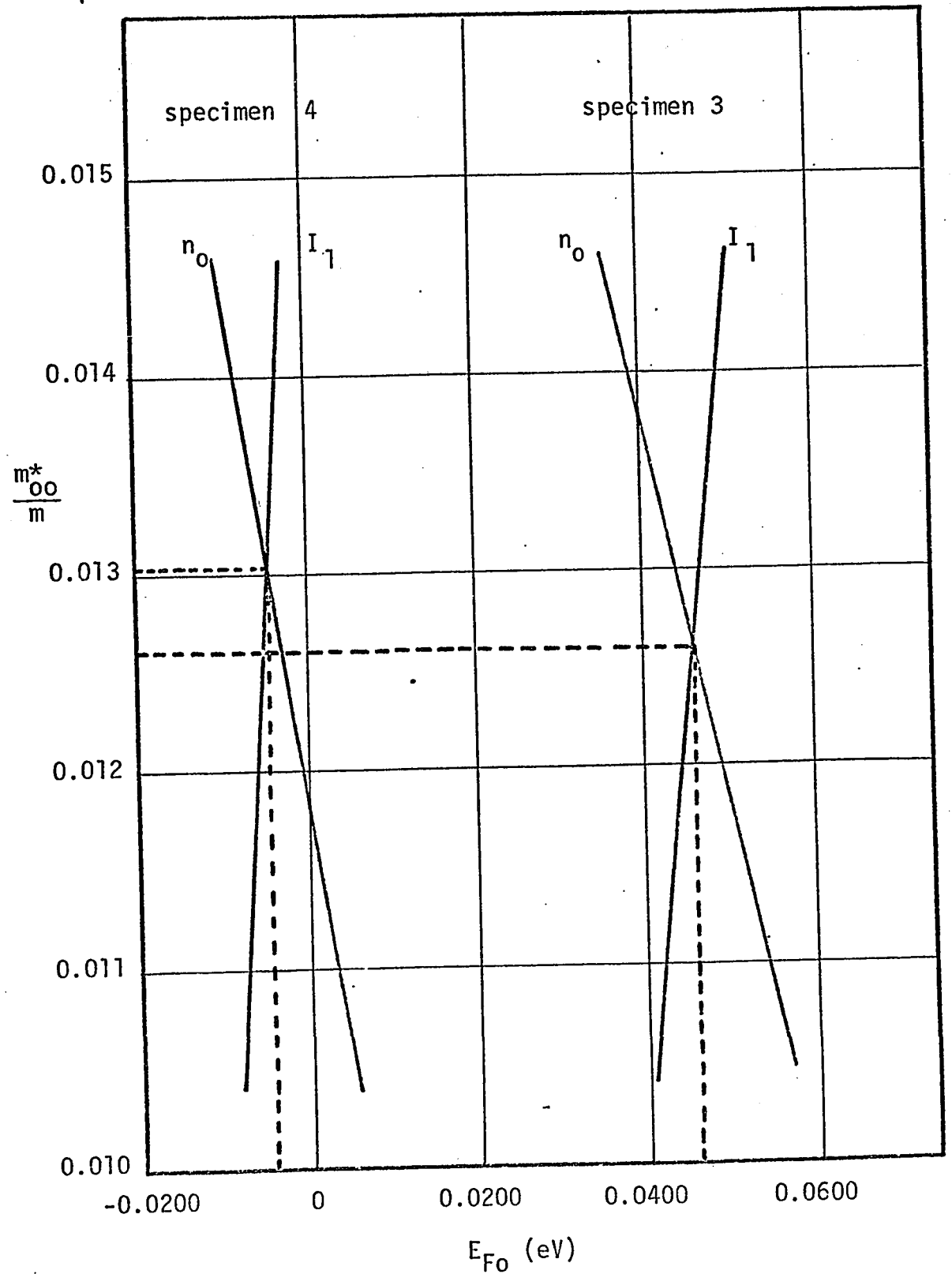


Fig. (5:2): Solutions of [2:37] and [2:38].

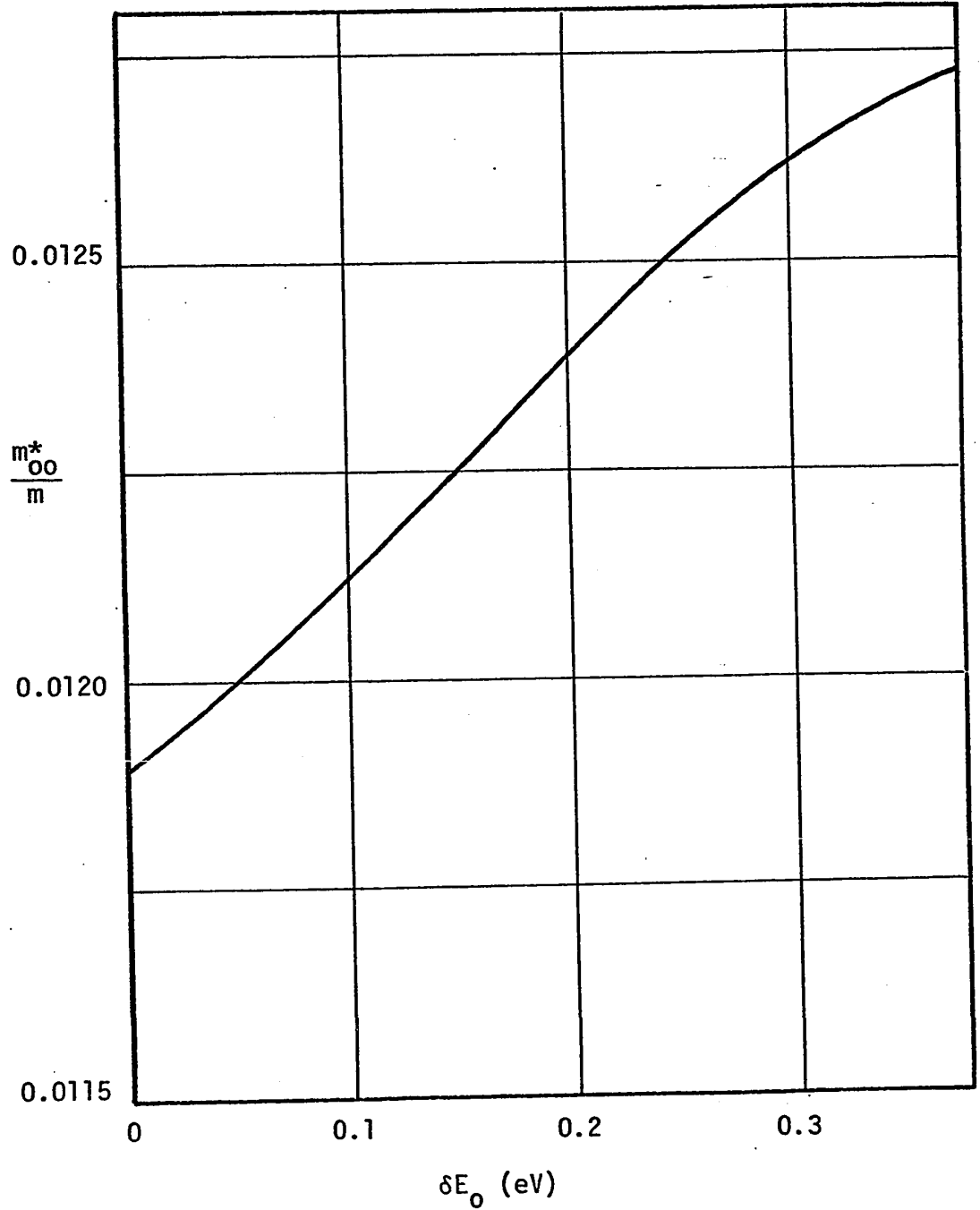


Fig. (5:3): Variation of $\frac{m_{co}^*}{m}$ with choice of δE_0 for specimen 3.

Using the values of $\frac{m_{00}^*}{m} = 0.013$ and $E_0^* = 0.21\text{eV}$ equation [2:38] and [2:40] can now be used to calculate the variations of E_{F0} and $\frac{m_{0F}^*}{m}$ with doping. These results are shown in figure (5: 4). The dashed curve represents the results obtained by using the degenerate analysis as in figure (5: 1). It can be seen that in the range $7 \times 10^{17}/\text{cc} < n_0 < 5 \times 10^{18}/\text{cc}$ the degenerate and non-degenerate analysis give the same results. At lower carrier concentrations the degenerate analysis is in error. At the higher carrier concentrations the Kane model is no longer applicable and here the degenerate analysis is expected to be more accurate. This, however, is some indication that the Kane model is a suitable choice for the carrier concentration range considered here.

In the variation of $\frac{m_{0F}^*}{m}$ with carrier concentration note that even at low carrier concentrations the effective mass does not reduce to the bottom of the band value of 0.013. This is because at room temperature in a semiconductor with such a small band gap $(0.18\text{eV})^{84}$ the thermal tail in the distribution of states function extends into the conduction band even when the Fermi level is in the center of the gap. Thus one would not expect any measurement to yield a value of 0.013 at room temperature.

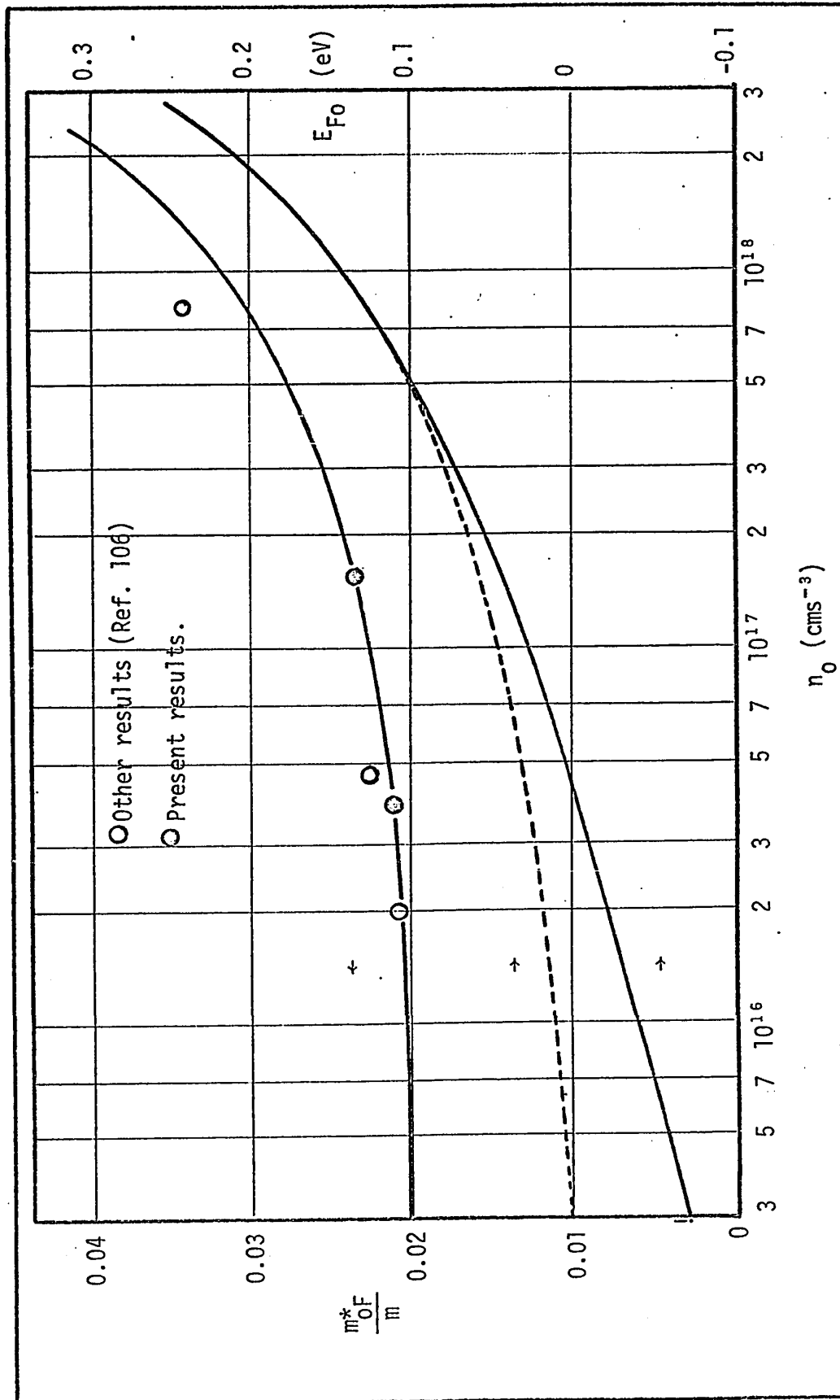


Fig. (5:4): Variation of Faraday effective mass and Fermi level with carrier concentration for InSb.

iv) GaAs and InAs

Measurements were made on specimen 5 and 6 in order to give some estimate of the value of cyclotron effective mass at the respective doping levels. These values were required for magnetoresistance and magneto-thermoelectric power measurements⁷².

Due to the relatively high carrier concentrations in these specimens the data were analysed using conditions (a) and (b). The results obtained were:

$$\text{At } n_0 = 3.95 \times 10^{18}/\text{cm}^3 \quad \frac{m_{oc}^*}{m} = .0788$$

$$\text{and at } n_0 = 8.32 \times 10^{17}/\text{cm}^3 \quad \frac{m_{oc}^*}{m} = .0686$$

Since the InAs data was analysed in the same way as the $\text{InSb}_{1-x}\text{As}_x$ alloys the results of these measurements is given in section (vi).

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Since the InAs data was analysed in the same way as the $\text{InSb}_{1-x}\text{As}_x$ alloys the results of these measurements is given in section (vi).

(v) GaSb

Recent measurements on the conduction bands of GaSb have been reported^{42,74,75}. In references 74 and 75 a simultaneous solution of 4.2°K magnetoresistance data from three differently doped specimen yielded values for ΔE , the energy separation of the (000) and <111> minima, and m_{1d}^*/m , the density of states effective mass of the electrons in the <111> minima. In this analysis it was assumed that the value of ΔE at any temperature was independent of the doping of the specimen. The values thus obtained were $\Delta E = 0.084\text{eV}$ at 4.2°K and $m_{1d}^*/m = 0.435$ while the value of $\frac{d}{dT} \Delta E$ was estimated to be $+ 8.1 \times 10^{-5}\text{eV}/^\circ\text{K}$.

In reference 42 the data from references 74 and 75 (i.e. $\Delta E = 0.0887\text{eV}$ at 77°K) were used to analyse Faraday rotation data and here a value of $m_{1d}^*/m = 0.293$ was found. One possible reason for the discrepancy between the two sets of results is indicated in a recent publication by Kwan and Woolley⁷⁸. Here magnetoresistance and other measurements on InAs indicate that for this compound the value of ΔE is very dependent on doping and thus it appears that the initial assumption in references 74 and 75, which is that ΔE is independent of the doping, is incorrect. Also in these references a very approximate form of the Kane model for the (000) conduction band was used and a value of the scattering parameter, $s = 1.5$, was arbitrarily chosen as the correct value at all temperatures.

In the present analysis the addition of Faraday rotation data at room temperature taken on the same specimens as in references 74 and 75,

allow the value of ΔE to be calculated for each sample and thus the variation of ΔE with doping can be investigated. Also a more accurate form of the Kane equation is used and the effect of the value of s is considered in more detail.

The detail of the procedure followed is given below. Since the value of ΔE is given by

$$\Delta E = (E_{F0} - E_{F1})$$

where E_{F0} and E_{F1} are the Fermi energies as measured from the (000) and $\langle 111 \rangle$ minima respectively, the analysis is directed towards finding these values.

The problem of analysing data on GaSb may be divided into two parts. Firstly the (000) constant energy surfaces are spherical and the (000) conduction band is non-parabolic. Secondly the $\langle 111 \rangle$ constant energy surfaces are ellipsoids of revolution and the $\langle 111 \rangle$ minima can be considered to be parabolic. The following steps show how the analysis is carried out.

a) A Kane model for the (000) conduction band is chosen. This involves knowing m_{00}^*/m and E_0^* . It can be shown that when $ak^2 \ll E$, which is valid for the specimens under consideration here, equation [2:36] reduces to

$$k = \left[\frac{E(E + E_0^*)}{aE_0^* \left(\frac{m}{m_{00}^*} - 1 \right)} \right]^{\frac{1}{2}} \dots\dots\dots [5:12]$$

For GaSb at room temperature¹⁸, $E_0^* = \frac{1}{2} (0.81 + 0.73) = 0.77\text{eV}$.

The value of m_{00}^*/m at room temperature can be estimated from the relation⁵⁸

$$m_{00}^*(T) = m_{00}^*(0) \frac{E_0^*(T)}{E_{00}} \dots\dots\dots [5:13]$$

Magneto-optical data⁴⁵ gives a value of $\frac{m_{00}^*}{m} (4.2^\circ\text{K}) = 0.047$ and hence $\frac{m_{00}^*}{m} (300^\circ\text{K}) = 0.0447$.

The carrier concentration, n_0 , in this band is given by [2:38].

For convenience when changing the integration variable to E this expression becomes

$$n_0 = \frac{(aE_0^* J)^{-\frac{3}{2}} I_3}{3\pi^2 kT} \dots\dots\dots [5:14]$$

where

$$I_3 = \int_0^\infty \frac{H^{\frac{3}{2}} dE}{G}$$

$$G = 2 + \exp \left[\frac{E - E_{Fo}}{kT} \right] + \exp \left[\frac{E_{Fo} - E}{kT} \right]$$

$$H = E(E + E_0^*)$$

$$J = \left(\frac{m}{m_{00}^*} - 1 \right)$$

and the energy dispersion relation is given by [5:12].

The Faraday rotation effective mass is given by [2:40] and on changing the integration variable again the relation becomes

$$\left(\frac{m_{OF}^*}{m}\right)^2 = \frac{I_3}{I_6} \dots\dots\dots[5:15]$$

where
$$I_6 = \int_0^\infty \frac{H^{\frac{3}{2}} \{1 + JL\}^2 dE}{G}$$

$$L = \{E_0^* / (2E + E_0^*)\}$$

and again [5:12] has been used.

It is therefore possible to calculate sets of values of n_0 , (m_{OF}^*/m) and E_{F0} which are consistent with [5:12].

(b) In a band of general shape, the Hall factor r_i is related to the relaxation times by

$$r_i = \langle (\tau_i / m_{ix}^*)^2 \rangle / \langle \tau_i / m_{ix}^* \rangle^2$$

where
$$\langle A_i \rangle = \frac{\int_0^\infty \frac{\partial f_0}{\partial E} A_i k^3 dE}{\int_0^\infty \frac{\partial f_0}{\partial E} k^3 dE}$$

and m_{ix}^* is an effective mass.

For the (000) conduction band m_{ox}^* lies somewhere between the cyclotron effective mass, m_{oc}^* , and the band curvature effective mass m_{ob}^* . Although the exact form of m_{ox}^* is not known, the analysis may be carried out with the assumptions that $m_{ox}^* = m_{oc}^*$ and $m_{ox}^* = m_{ob}^*$ as limiting cases.

The relaxation times can be related to the band structure by⁸³

$$\tau = \text{Const.} \times k^{2s-1} \frac{dE}{dk}$$

and thus for the (000) band the Hall factor is given by

$$r_o = \frac{\int_0^\infty \frac{\partial f_o}{\partial E} k^{4s+1} \left[\frac{dE}{dk} \right]^{4-2p} \left[\frac{d^2E}{dk^2} \right]^{2p} dE \int_0^\infty \frac{\partial f_o}{\partial E} k^3 dE}{\left[\int_0^\infty \frac{\partial f_o}{\partial E} k^{2s+2} \left[\frac{dE}{dk} \right]^{2-p} \left[\frac{d^2E}{dk^2} \right]^p dE \right]^2} \dots\dots\dots [5:16]$$

where the factor p signifies the use of the cyclotron effective mass ($p = 0$) or the band curvature effective mass ($p = 1$) and s depends on the relevant scattering mechanism. Using [5:12] in [5:16] the resultant expression is

$$r_o = \frac{I_3 I_5}{(I_4)^2} \dots\dots\dots [5:17]$$

where
$$I_4 = \int_0^\infty \frac{H^s + \frac{3}{2} \{1 + JL\}^{2-p} \{1 + JL^3\}^p dE}{G}$$

and
$$I_5 = \int_0^\infty \frac{H^{2s + \frac{3}{2}} \{1 + JL\}^{4-2p} \{1 + JL^3\}^{2p} dE}{G}$$

For each sample the analysis is thus carried out for different sets of (p, s) which are (0,0.0), (0,0.5), (0,1.0), (0,1.5), (1,0.0), (1,0.5), (1,1.0) and (1,1.5).

With each of these sets, consistent values for r_0 , n_0 , m_{0F}^*/m and E_{F0} are calculated at this stage. In order to decide which of these values is correct the value of $n_0/r_0 F_0$ from Table 4E is used. Since the (000) constant energy surfaces are spherical, as mentioned in Chapter one, $K_0 = 1.0$ and hence from equation [3:2], $F_0 = 1.0$. The experimental value of n_0/r_0 will thus indicate which values of E_{F0} , m_{0F}^*/m and therefore n_0 and r_0 are correct for each set of (p, s).

(c) To a reasonable approximation the <111> minima may be treated as parabolic. Under this condition r_1 is given by

$$r_1 = \frac{3(2s + 3/2) F_{\frac{1}{2}} (E_{F1}/kT) F_{2s + \frac{1}{2}} (E_{F1}/kT)}{2(s + 3/2)^2 \left\{ F_s + \frac{1}{2} (E_{F1}/kT) \right\}^2} \dots\dots\dots [5:18]$$

where F_q is defined by [2:41] or by $q(kT)^q F_{q-1}(E_{F1}/kT) = \int_0^\infty \frac{\partial f_0}{\partial E} E^q dE$.

There are accurate tables for these functions calculated by Coderre¹⁸.

The carrier concentration is related to the Fermi energy by [2:43]. The multiplicity of these minima is four and on using [1:10] the relation becomes

$$n_1 = (1/2\pi^2)(kT/a)^{\frac{3}{2}} 4K_1^{\frac{1}{2}} (m_{1c}/m)^{\frac{3}{2}} F_{\frac{1}{2}}(E_{F1}/kT) \dots \dots [5:19]$$

In order to solve for r_1 , n_1 , and E_{F1} the experimental value of $n_1/r_1 F_1$ is needed. K_1 is taken to be⁸² 8.6 and thus $F_1 = 0.83$. The solution of [5:18] and [5:19] is now found by choosing a value for s as in the case of the (000) band and using a starting value for m_{1c}/m . This yields a set of values for n_1 , r_1 , E_{F1} and of course m_{1c} .

(d) The results obtained from (b) and (c) are fed into equation [5:11] remembering that here $m_{OR}^*/m = m_{OF}^*/m$ since $K_0 = 1$ and the values of η are calculated at the wavelengths at which the Faraday rotation was measured. Equation [5:10] is then curve fitted by a least squares method using the data in figure [4:4]. The fitted equation is of the form

$$\theta\eta = A\lambda^2 + B'\frac{\eta}{\lambda^2}$$

where the coefficient A represents the free carrier effect only. Once

this coefficient has been found m_{1x} is calculated from it using the values of n_0 , m_{OF}^*/m and n_1 . If this new value is not the same as the initial value of m_{1x} this starting value is increased and fed into section (c). This procedure is repeated until the final calculated value of m_{1x} and the starting value are the same. Here then a consistent set of solutions for n_0 , n_1 , r_0 , r_1 , E_{F0} , E_{F1} , m_{OF}^*/m and m_{1x}/m are found for each set of (p, s) for each specimen.

The program for this calculation can be found in the appendix. The tabulated results are given in Tables 5B and 5C. The column headed atomic % Te is calculated from the values of $(n_0 + n_1)$ and the assumption that all the tellurium atoms are ionized.

In Table 5C note that for some specimen no solution could be found for $s = 1.5$. This is because the calculated contribution of the (000) electrons to the free carrier rotation was larger than the total rotation measured. However, measurement of magneto-thermoelectric power on various III-V materials⁸¹ show that for samples with values of n_0 and n_1 such as those used here (i.e. $20 \times 10^{16}/\text{cm}^3$ to $400 \times 10^{16}/\text{cm}^3$), the appropriate value of s lies between 0.5 and 1.0. Hence a value of $s = 1.5$ might be expected to give anomalous results in this analysis.

Since the $\langle 111 \rangle$ band will show little deviation from parabolic form over the energy range considered here, for the correct value of s , the calculated variation of m_{1x}/m from one specimen to another should be

(p, s)	Spec #	r_0	r_1	n_0 ($\times 10^{16}/\text{cm}^3$)	n_1 ($\times 10^{16}/\text{cm}^3$)	$n_0 + n_1$ ($\times 10^{16}/\text{cm}^3$)	At%Te y	E_{Fo} (eV)	E_{F1} (eV)	ΔE (eV)	$\frac{m_{OF}^*}{m}$	$\frac{m_{12}}{m}$
(0,0.0)	7	1.02	1.00	59.4	207.5	266.9	.0075	.0360	-.0299	.0659	.0538	.087
	8	1.02	1.00	29.4	90.9	120.3	.0034	.0098	-.0567	.0665	.0527	.097
	9	1.02	1.00	8.1	17.2	25.3	.0007	-.0292	-.0956	.0660	.0518	.086
	10	1.02	1.00	16.8	39.3	56.1	.0016	-.0081	-.0727	.0646	.0522	.089
(1,0.0)	7	1.09	1.00	63.2	207.5	270.7	.0076	.0386	-.0323	.0709	.0540	.092
	8	1.09	1.00	31.2	90.9	122.1	.0034	.0118	-.0598	.0716	.0528	.105
	9	1.09	1.00	8.6	17.2	25.8	.0007	-.0275	-.0991	.0716	.0518	.095
	10	1.09	1.00	17.8	39.3	57.1	.0016	-.0063	-.0770	.0707	.0522	.093
(0,0.5)	7	1.01	1.10	58.9	227.3	286.2	.0081	.0356	-.0293	.0649	.0538	.091
	8	1.02	1.10	29.3	100.1	129.4	.0036	.0097	-.0561	.0658	.0527	.102
	9	1.03	1.10	8.2	19.0	27.2	.0008	-.0290	-.0949	.0659	.0518	.091
	10	1.03	1.10	16.8	43.3	60.1	.0017	-.0081	-.0727	.0646	.0522	.089
(1,0.5)	7	1.01	1.10	58.4	227.3	285.7	.0080	.0353	-.0288	.0641	.0538	.090
	8	1.01	1.10	28.9	100.1	129.0	.0036	.0092	-.0554	.0646	.0527	.100
	9	1.01	1.10	8.0	19.0	27.0	.0008	-.0296	-.0936	.0640	.0518	.088
	10	1.01	1.10	16.5	43.4	59.9	.0017	-.0086	-.0716	.0632	.0532	.087

T A B L E 5B

(p, s)	Spec #	r_o	r_l	n_o ($\times 10^{16}/\text{cm}^3$)	n_l ($\times 10^{16}/\text{cm}^3$)	$n_o + n_l$ ($\times 10^{16}/\text{cm}^3$)	At%Te y	E_{Fo} (eV)	E_{Fl} (eV)	ΔE (eV)	$\frac{m_{OF}^*}{m}$	$\frac{m_l}{m}$
(0,1.0)	7	1.12	1.37	65.0	284.3	349.3	.0098	.0398	-.0317	.0715	.0541	.112
	8	1.16	1.39	33.4	126.4	159.8	.0045	.0142	-.0628	.0770	.0529	.141
	9	1.21	1.40	9.6	24.1	33.7	.0009	-.0244	-.1086	.0842	.0519	.152
	10	1.12	1.40	19.5	54.9	74.4	.0021	-.0035	-.0829	.0784	.0523	.132
(1,1.0)	7	1.05	1.37	60.7	283.7	344.4	.0097	.0369	-.0291	.0660	.0539	.105
	8	1.07	1.39	30.7	126.1	156.8	.0044	.0113	-.0571	.0684	.0528	.122
	9	1.10	1.40	8.7	24.1	32.8	.0009	-.0272	-.0979	.0707	.0518	.115
	10	1.09	1.39	17.8	54.8	72.6	.0020	-.0064	-.0749	.0685	.0522	.110
(0,1.5)	7	1.34	1.88	77.5	390.2	467.7	.0134	.0475	-.0402	.0877	.0545	.170
	8											
	9											
	10											
(1,1.5)	7	1.18	1.86	68.5	368.8	437.3	.0128	.0420	-.0325	.0745	.0542	.140
	8	1.25	1.91	35.9	174.0	209.9	.0059	.0167	-.0684	.0850	.0530	.201
	9											
	10	1.30	1.92	21.2	75.7	96.9	.0027	-.0009	-.0920	.0911	.0524	.212

T A B L E 5C

small and any variation observed should be of m_{1x}/m increasing as the carrier concentration n_1 increases. In the values of m_{1x}/m tabulated in Tables 5B and 5C it is seen that for $s = 1.5$, the variation in m_{1x}/m was large and that m_{1x}/m tended to decrease with increasing carrier concentration. However, for $0 \leq s \leq 1.0$ the values of m_{1x}/m were fairly constant, any variation in m_{1x}/m being due to experimental scatter. From this data, it appears that the correct value of s lies in the range $0 \leq s \leq 1.0$, while the magneto-thermoelectric power data indicate a value in the range $0.5 \leq s \leq 1.0$. For each s in the range of interest the appropriate value of m_{1x}/m has been taken as the mean over the values for the four specimens 7, 8, 9 and 10.

The data in Tables 5B and 5C also shows the variation of m_{0F}^*/m with carrier concentration. This is shown in figure (5: 5). For GaSb this variation seems to be almost linear over the concentration range under consideration and at most is about 10% when the carrier concentration changes from $10^{17}/\text{cm}^3$ to $10^{18}/\text{cm}^3$.

In order to investigate the variation of ΔE with tellurium content the values of ΔE vs the atomic % of tellurium are plotted in figure (5: 6) for each set of $(p, s, m_{1x}/m)$. Here, as mentioned before, the value of m_{1x}/m is taken as the mean over the values of the four specimens. There is some experimental scatter associated with this plot. The lines drawn are obtained from a least squares fit of the

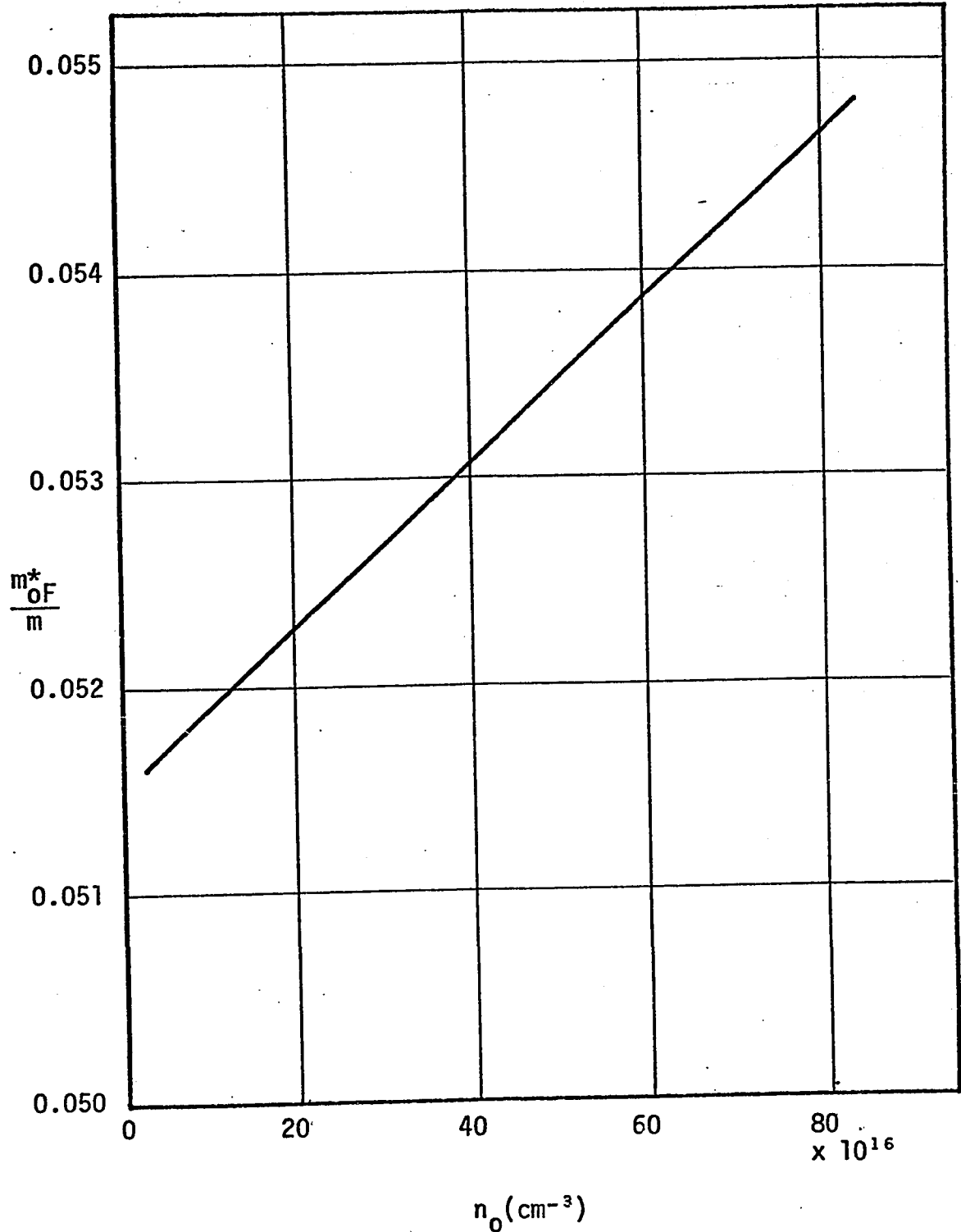


Fig. (5:5): Variation of Faraday effective mass with carrier concentration at room temperature for GaSb.

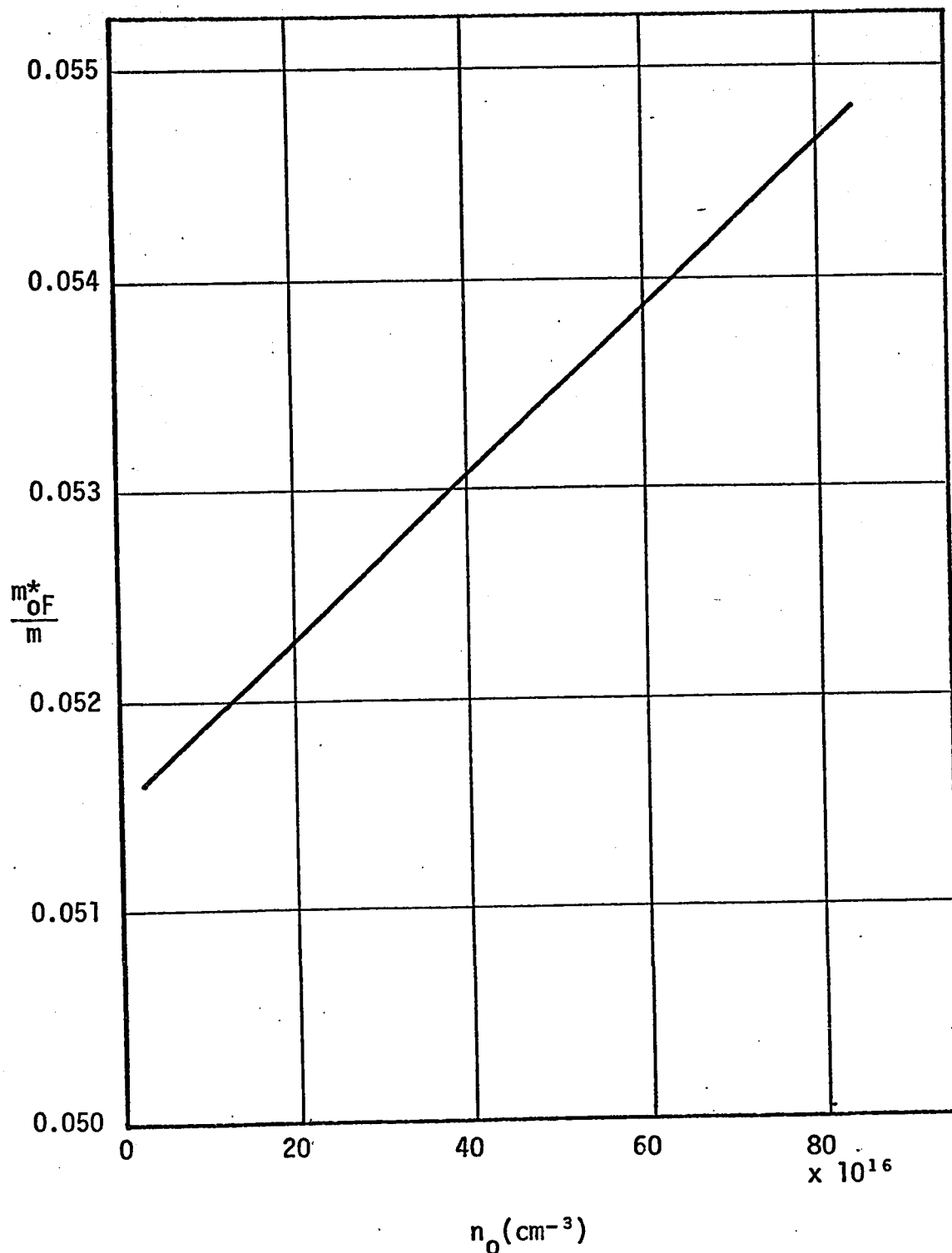
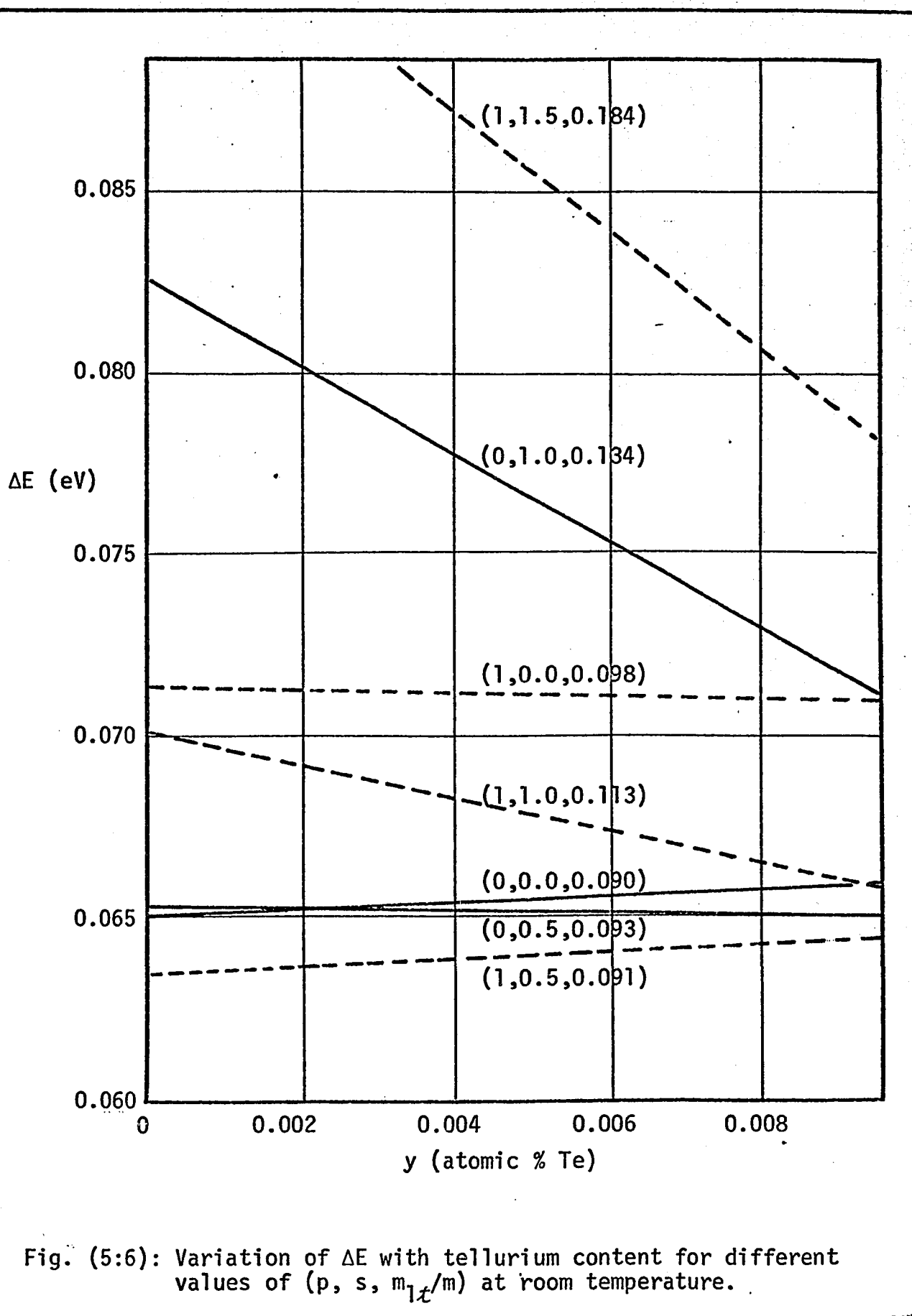


Fig. (5:5): Variation of Faraday effective mass with carrier concentration at room temperature for GaSb.



data. The variation of ΔE with the doping is very dependent on the choice of (p, s) and hence at this stage nothing more can be said about the results.

e) Further analysis now requires the use of the magneto-resistance data at 4.2°K given in references 74 and 75. In the initial analysis of this data, both m_{1x}/m , p and s must be treated as unknowns. Assuming in this case $m_{00}^*/m = 0.047$ and $E_0^* = 0.81$ eV and using the appropriate value of $n_0/r_0 F_0$ and $n_1/r_1 F_1$ for samples 6, 7 and 7A given in these references equations [5:14], [5:17], [5:18] and [5:19] are solved to give consistent sets of values of r_0 , r_1 , n_0 , n_1 , E_{F0} , E_{F1} and ΔE_0 (ΔE_0 is the value of ΔE at 4.2°K) for each choice of m_{1x}/m at a set of (p, s) . However at this low temperature, it was found that the results of this analysis were completely independent of p or s . This is to be expected since because of the degeneracy of the specimens at 4.2°K, ($E_{F1} \gg kT$), the integrals in the evaluation of r_0 are different from zero only at the Fermi level and hence $r_0 = r_1 = 1.0$ at 4.2°K for each choice of p and of s .

Thus, the band gap ΔE_0 can be treated as a function of m_{1x}/m only, and for each specimen (6, 7 and 7A) the calculated variation of ΔE_0 with m_{1x}/m is shown in fig. (5: 7). Some other results are shown in Table 5D .

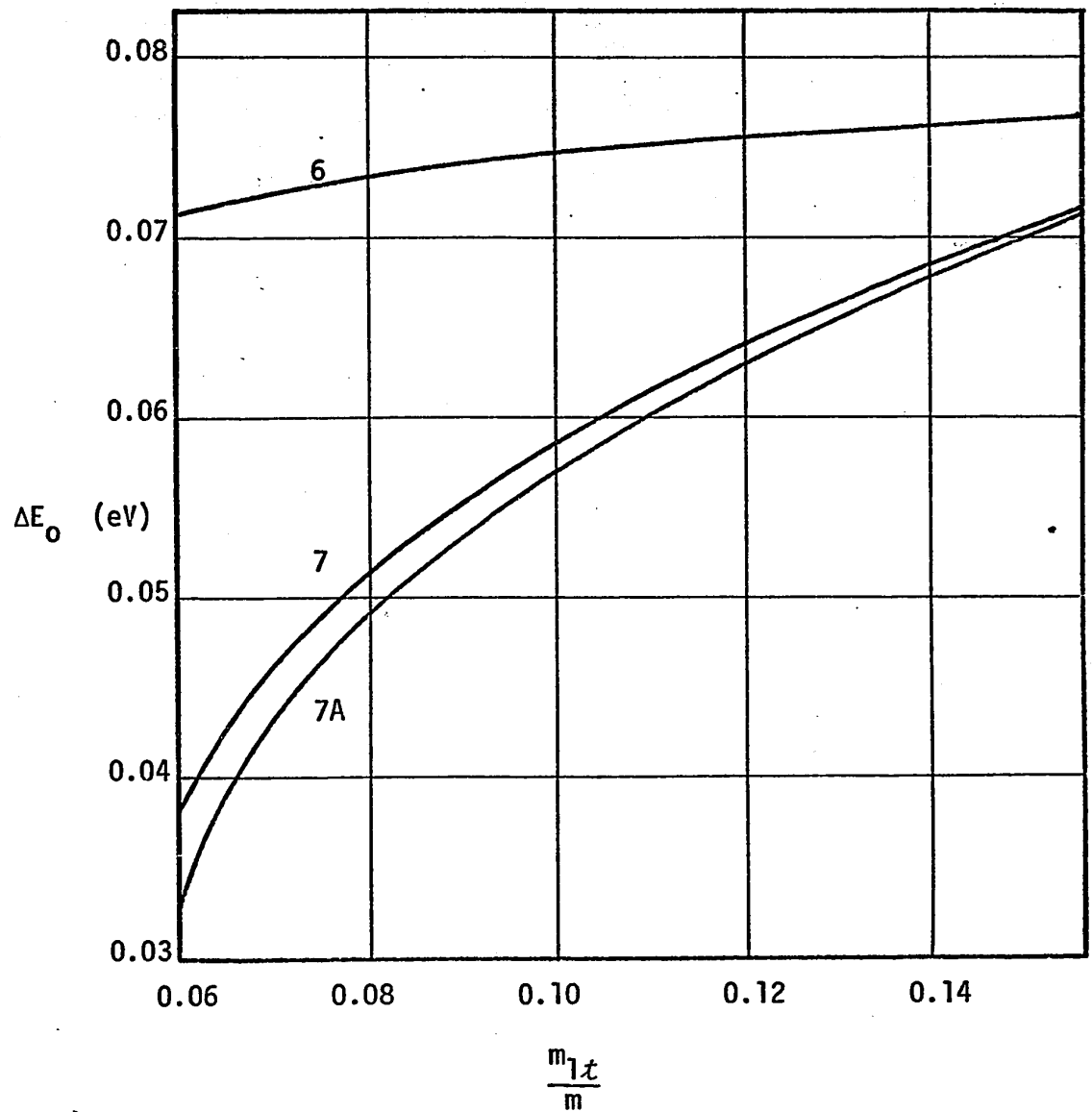


Fig. (5:7): Calculated variation of ΔE_0 with $m_1 x/m$ for specimens 6, 7, 7A of references 74 and 75.

Specimen number Ref. 74&75	n_0 ($\times 10^{16}/\text{cm}^3$)	n_1 ($\times 10^{16}/\text{cm}^3$)	$n_0 + n_1$ ($\times 10^{16}/\text{cm}^3$)	At.%Te y
6	130	60	190	.0053
7	160	954	1,114	.0314
7A	164	1095	1,259	.0354

T A B L E 5D

In order to investigate the variation of ΔE_0 with tellurium content the values of ΔE_0 at a chosen value of m_{1x}/m is plotted against the atomic % of tellurium in each specimen. This variation is shown in fig. (5: 8) for different values of m_{1x}/m .

These graphs appear linear within the limits of experimental error, and extrapolation to $y = 0$ should give the value of ΔE_0 for intrinsic GaSb. It is seen that the lines for the different values of m_{1x}/m all extrapolate to the same value of $\Delta E_{00} = 0.078$ eV. Hence, this would appear to be the correct band separation for intrinsic GaSb at 4.2°K and the value obtained is independent of the choice of (p, s) or m_{1x}/m .

In order to find the values of m_{1x}/m , $\frac{d}{dy} \Delta E$ and $\frac{d}{dT} \Delta E$ it is necessary to assume that m_{1x}/m and $\frac{d}{dy} \Delta E$ are temperature independent.

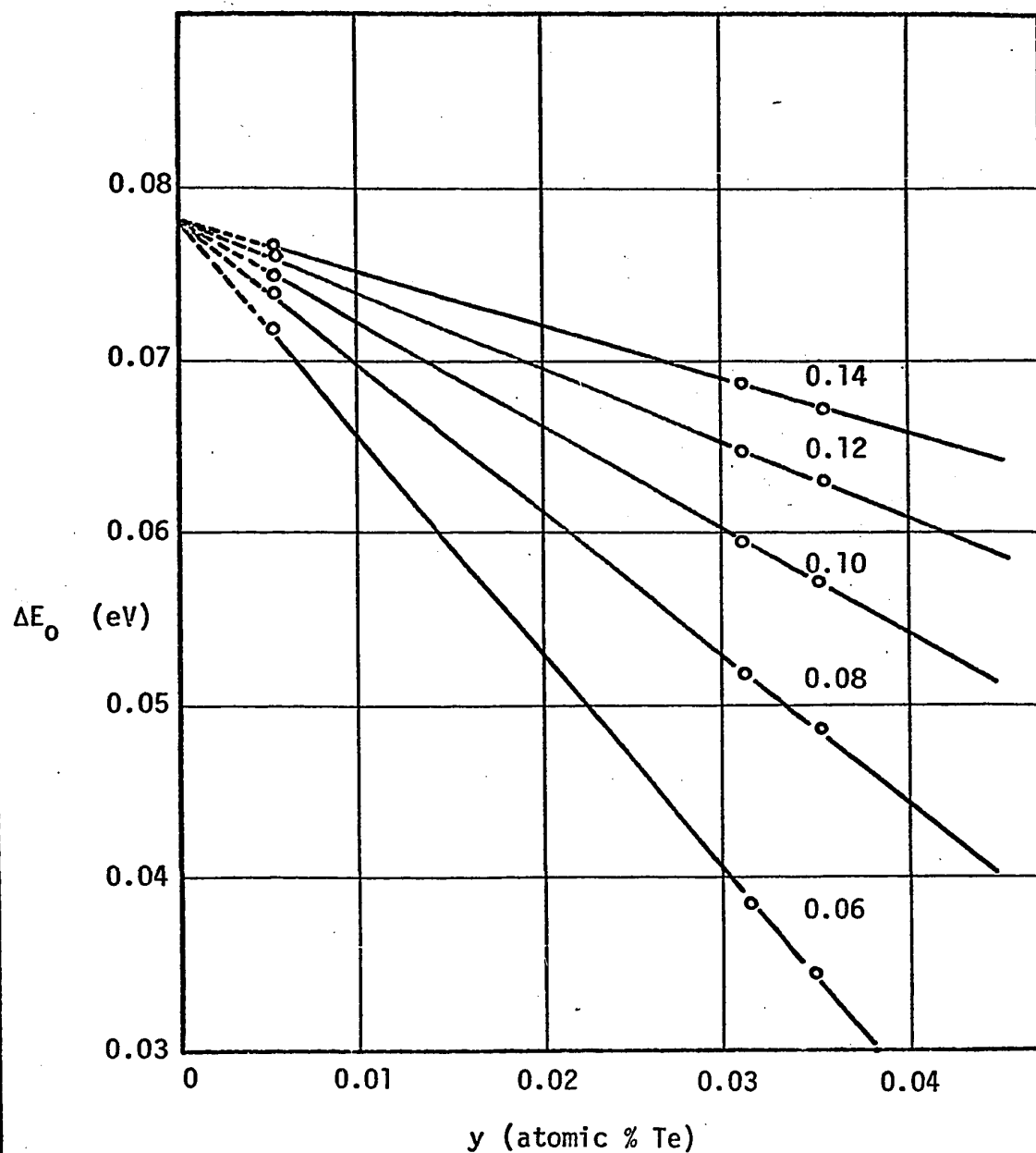


Fig. (5:8): Variation of ΔE_0 with tellurium content for different m_h/m at 4.2°K.

These assumptions are not too drastic since the $\langle 111 \rangle$ minima for GaSb are quite far in energy from the valence band at room temperature and hence the interaction between these two bands is not too temperature dependent. The factor m_{1x}/m which is in fact a measure of this interaction can thus be considered to be constant. Also since the variation of ΔE with tellurium content is purely a crystallographic effect $\frac{d}{dy} \Delta E$ can to a first approximation be taken as being constant with temperature.

In figure (5: 9) the variation of $\frac{d}{dy} \Delta E$ with m_{1x}/m is shown for the 4.2°K and room temperature results.

The curves at room temperature are different for $p = 0$ and $p = 1$. However, since as has been mentioned these values of p refer to limiting cases only as the correct form of m_{ox}^* was not known. The point giving $m_{1x}/m = 0.11$ and $\frac{d}{dy} \Delta E = -0.5 \text{ eV/at. \% Te}$ is therefore taken to be the common solution between the room temperature and 4.2°K results. For $p = 0$ the intersection is at $s = 0.75$ and for $p = 1$, $s = 1.0$. These values of s are consistent with the results of magneto-thermoelectric power measurements on various III-V materials⁸¹.

Using the values $p = 1$, $s = 1.0$ and referring back to fig. (5: 6) the room temperature value of ΔE is 0.070eV. The temperature dependence of this separation is thus seen to be $-3 \times 10^{-5} \text{ eV/°K}$ but this is a rough estimate only

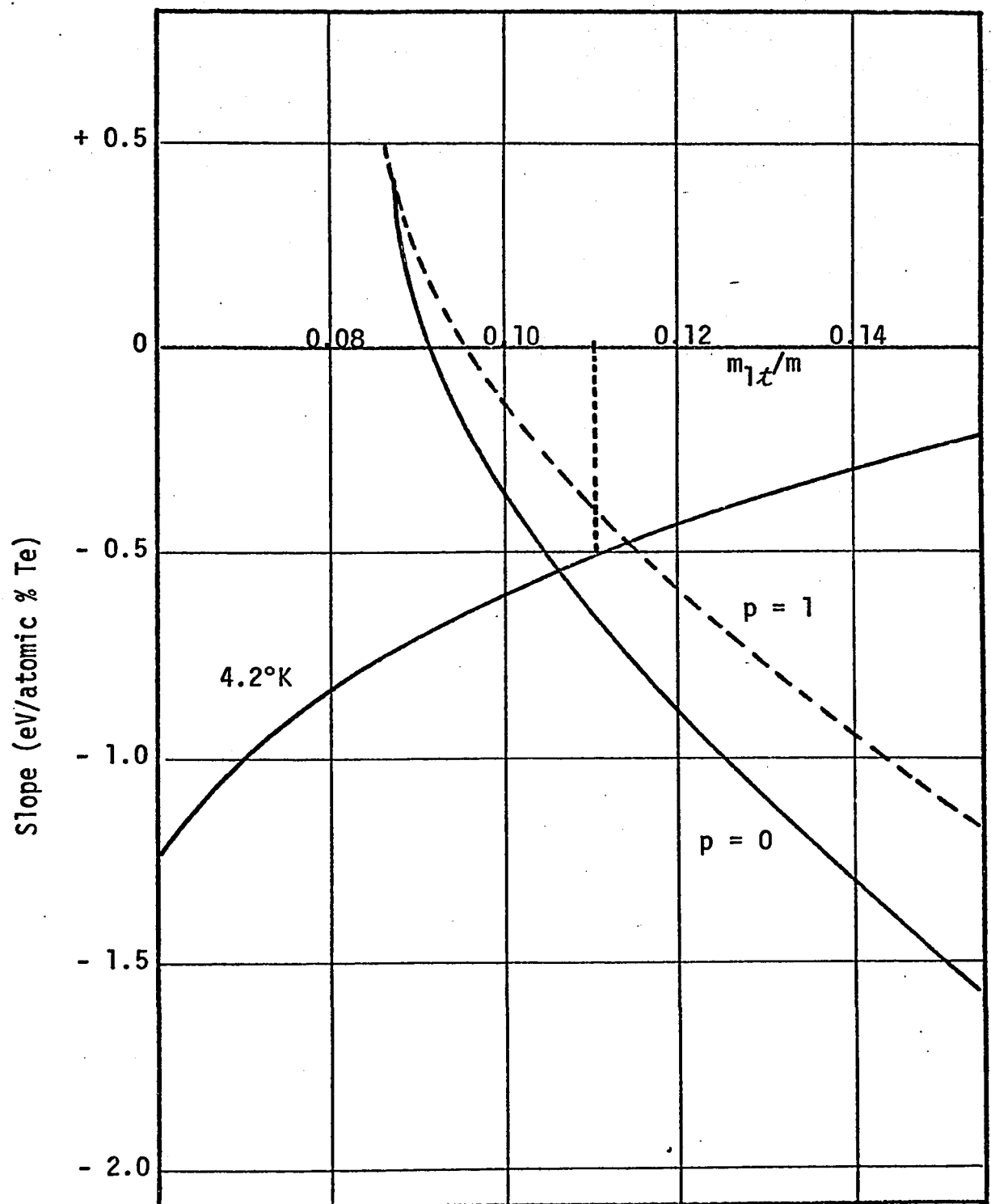


Fig. (5:9): Variation of the slope with $m_1 t / m$ at room temperature and 4.2°K .

vi) $\text{InSb}_{1-x}\text{As}_x$

The doping levels of these specimens were relatively low and hence these data were analysed using conditions (a) and (c) in section (ii) of this chapter. The variation of the refractive index was found to be small and hence corrections to n were not necessary. The values of ϵ_r for InSb and InAs are 16.8 and 11.6 respectively⁸⁶. It has been shown^{87,88} that, for a similar alloy system, $\epsilon_r^{\frac{1}{2}}$ varies linearly with x . Hence in this case a linear variation of the refractive index with x between 3.41 and 4.10 has been assumed. In the analysis of this data the variation of $E_0^* = \frac{1}{2} (E_{00} + E_0)$ with composition was taken from the optical absorption data of Woolley and Warner²⁸, (E_0) , and the Hall coefficient data of Coderre and Woolley⁸⁵, E_{00} .

Using the technique described in (ii)(c) of this chapter the results tabulated in Table 5E were obtained.

The variation of m_{00}^*/m as a function of x is shown in figure (5:10) together with the results of magneto-thermoelectric power measurements of Aubin and Woolley⁴⁷ these latter again using the above assumption about E_0^* . It is seen that the two sets of data show very good agreement.

An attempt was made to analyse the thermoelectric power data in order to find separately, a value for the Fermi level. These measurements were analysed using the relation⁸⁹

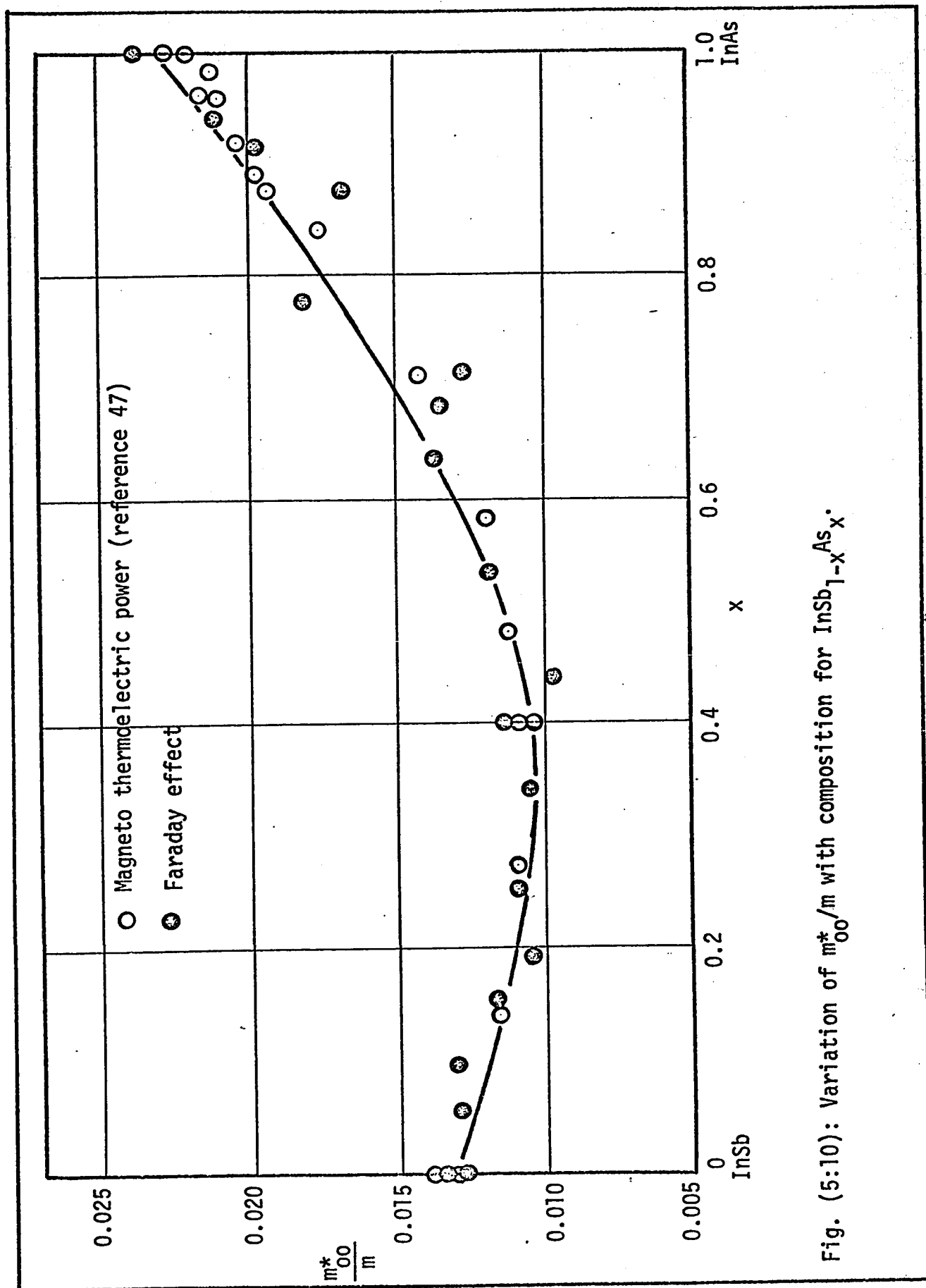


Fig. (5:10): Variation of m_{00}^*/m with composition for $\text{InSb}_{1-x}\text{As}_x$.

Specimen number	x	I_1 ($\times 10^{-9}(\text{eV})^2\text{m}$)	E_0^* (eV)	E_{F0} (eV)	m_{00}^*/m
3	0	0.2116	0.210	0.0465	0.0126
4	0	0.0608	0.210	-0.0043	0.0131
12	0.090	0.6930	0.179	0.0016	0.0128
13	0.150	0.0910	0.163	0.0111	0.0116
14	0.190	0.1067	0.155	0.0160	0.0103
15	0.250	0.1341	0.146	0.0275	0.0106
16	0.340	0.1230	0.137	0.0236	0.0101
17	0.400	0.1440	0.134	0.0334	0.0111
18	0.440	0.1480	0.134	0.0311	0.0094
19	0.535	0.1371	0.144	0.0298	0.0112
20	0.635	0.1098	0.167	0.0201	0.0128
21	0.680	0.1204	0.184	0.0220	0.0126
22	0.710	0.1818	0.199	0.0382	0.0119
23	0.775	0.0801	0.235	0.0087	0.0175
24	0.870	0.2243	0.302	0.0490	0.0165
25	0.910	0.1262	0.333	0.0240	0.0195
26	0.935	0.1481	0.350	0.0319	0.0210
27	0.960	0.0672	0.369	0.0010	0.0211
11	1.000	0.0245	0.408	-0.0287	0.0242

T A B L E 5E

$$\alpha = -\frac{k}{e} \left[\frac{(s + \frac{3}{2}) \frac{kT}{E_0^*} F_s + \frac{5}{2} \left\{ \frac{E_{F0}}{kT} \right\} + (s + \frac{5}{2}) F_s + \frac{3}{2}}{(s + \frac{5}{2}) \frac{kT}{E_0^*} F_s + \frac{3}{2} \left\{ \frac{E_{F0}}{kT} \right\} + (s + \frac{3}{2}) F_s + \frac{1}{2}} - \frac{E_{F0}}{kT} \right]$$

It was found, however, that the value of the Fermi level was very dependent on the choice of s . Furthermore, when E_{F0} values are taken from Table 5E and inserted into the above equation, s values in the range $-0.2 < s < 0.7$ are found. These measurements were therefore not very useful in giving any extra information.

In the analysis of previous measurements of Faraday rotation on InSb⁵⁰ and InAs⁹⁰ a different form of the Kane equation was used. Here the parameters in the conduction band model were E_0^* and P^2 , the momentum matrix element. As can be seen from equation [2:34] these quantities are related to m_{00}^*/m . Hence, in the present analysis values for P^2 can be calculated if Δ_0 , the spin-orbit splitting of the valence band is known.

Using the values of m_{00}^*/m given by the curve in figure (5:10), values of P^2 have been calculated from equation [2:34] assuming that Δ_0 varies linearly from 0.82eV for InSb⁹¹ to 0.38eV for InAs⁹². These values are shown in fig. (5:11). It is seen that a value of $P^2 \approx 21\text{eV}$ (0.39 atomic units) is obtained for both InSb and InAs and that for the alloys P^2 shows a shallow minimum of 18eV (0.33 a.u.) at about $x = 0.4$.

The accuracy of these values of P^2 depends upon the correct choice of E_0^* and upon the accuracy of the values of m_{00}^*/m . Systematic errors may

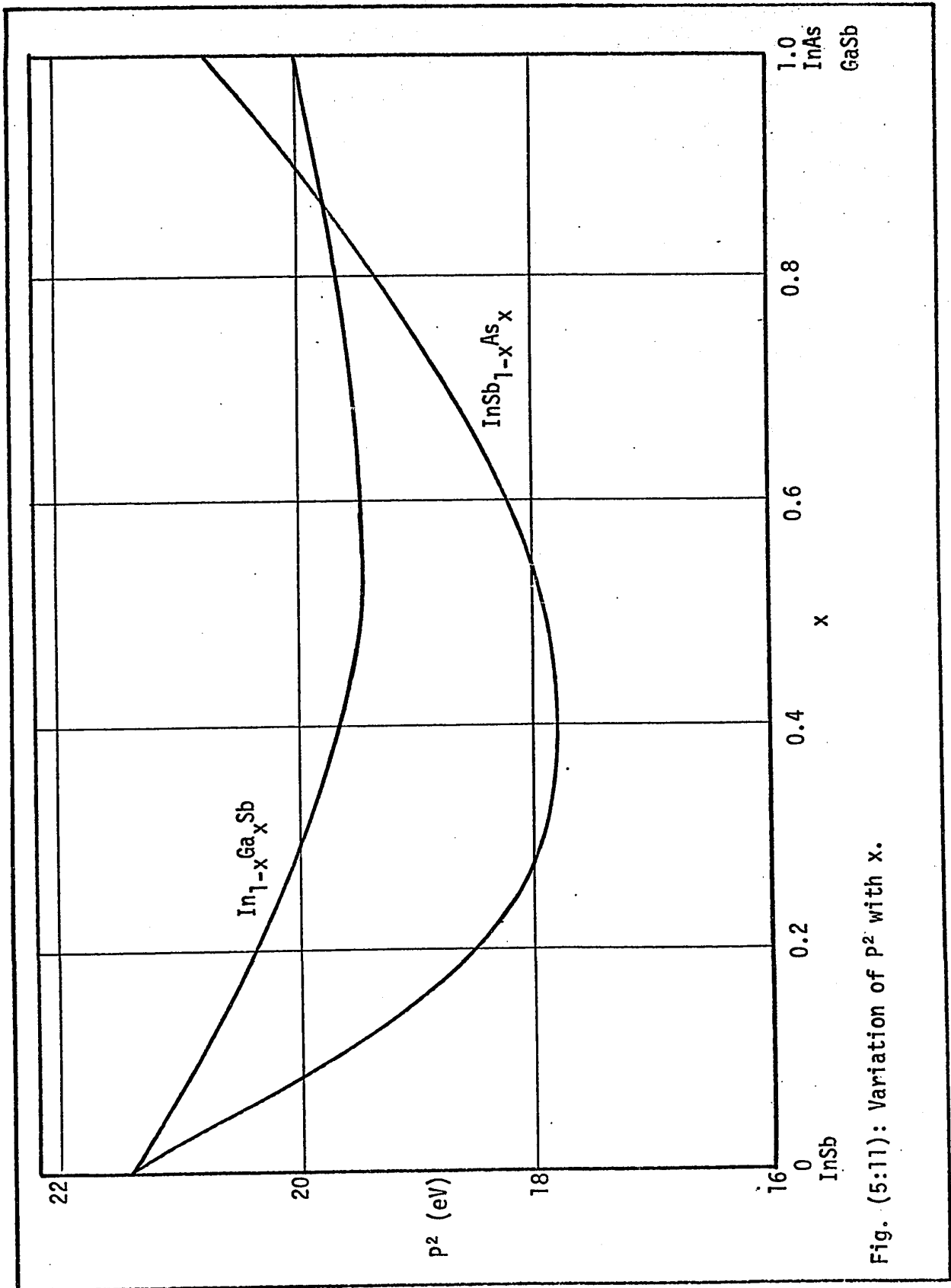


Fig. (5:11): Variation of P^2 with x .

be present in the latter values, owing to the choice of the Kane equation and to the values of E_0^* used. These effects may tend to cancel one another, however, since the assumed form of δE_0 is taken from the results for InSb⁵⁰, where E_0^* was effectively an adjustable parameter applied to the simple Kane equation. Estimates using a more accurate form of Kane equation⁹³ would indicate that the systematic error due to the choice of the band model should not exceed about 5% for the Fermi energies found here. Since P^2 is much more sensitive to the choice of E_0^* than is m_{00}^*/m the form of the P^2 vs x curve gives some indication of the suitable choice of E_0^* . The values of P^2 for the compounds are in good agreement with the values given in reference 50 (InSb, $P^2 = 0.395$ a.u., 21.5eV), by Pidgeon et. al.⁹⁴ (InAs, $P^2 = 0.38$ a.u., 20.7eV) and in reference 90 (InAs, $P^2 = 0.36$ a.u., 19.6eV). The curve in figure (5:11) shows a simple curvature of the form to be expected in alloys, and it is impossible to raise this into a value independent of x without assuming for the alloys close to $x = 0.4$ values of E_0^* well outside the E_0 to E_{00} range.

Summers and Smith⁹⁰ have stated that to fit their Faraday rotation data for InAs, a value of $E_0^* = E_0$ had to be assumed. However, it was found with the present results that, if such a value of E_0^* was assumed for InAs, a value of 18eV was obtained for P^2 , which is considerably lower than the previous values. Since the value of $E_0^* = \frac{1}{2} (E_{00} + E_0)$

gives satisfactory values for P^2 for the compounds it is felt that this choice is suitable.

vii) $\text{In}_{1-x}\text{Ga}_x\text{Sb}$

The specimens cut from ingot DF-A-8 were found to be relatively highly doped. For this reason corrections to η due to free carrier effects must be taken into consideration. These doping levels, however, do not justify the use of the complete degeneracy equations and hence the analysis technique outlined in section (ii)(c) was used. The results of this analysis is shown in Table 5F. The values E_0^* are taken from the results of optical absorption experiments^{95,96,97}, (E_0), and the electrical measurements of Coderre¹⁸, (E_{00}). The variation of m_{00}^*/m with x is shown in fig. (5:12) together with the results from magneto-thermoelectric power measurements⁸¹ and the results of infrared reflectivity measurements⁸¹. In all the analyses the same definition for E_0^* was used and the agreement between the results of these different measurements is seen to be very good. In the range of high x values, no data is given since here the (000) and $\langle 111 \rangle$ minima get very close in energy^{18,76} and the analysis on single specimen measurements, becomes intractable.

In order to estimate from the Kane equation, more accurate values of P^2 corresponding to the present $\frac{m_{00}^*}{m}$ values it is necessary to know the value of Δ_0 for this system. Here then Δ_0 has been taken to be 0.82eV for all the alloys since this is the accepted value for InSb⁹¹, while that for GaSb is very close to this value⁹⁸. Values of P^2 have been calculated corresponding to the smooth curve in fig. (5:12). This gives a value of about 21eV at InSb and 20eV at GaSb while again the values for the alloys

vii) $\text{In}_{1-x}\text{Ga}_x\text{Sb}$

The specimens cut from ingot DF-A-8 were found to be relatively highly doped. For this reason corrections to η due to free carrier effects must be taken into consideration. These doping levels, however, do not justify the use of the complete degeneracy equations and hence the analysis technique outlined in section (ii)(c) was used. The results of this analysis is shown in Table 5F. The values E_0^* are taken from the results of optical absorption experiments^{95,96,97}, (E_0), and the electrical measurements of Coderre¹⁸, (E_{00}). The variation of m_{00}^*/m with x is shown in fig. (5:12) together with the results from magneto-thermoelectric power measurements⁸¹ and the results of infrared reflectivity measurements⁸¹. In all the analyses the same definition for E_0^* was used and the agreement between the results of these different measurements is seen to be very good. In the range of high x values, no data is given since here the (000) and $\langle 111 \rangle$ minima get very close in energy^{18,76} and the analysis on single specimen measurements, becomes intractable.

In order to estimate from the Kane equation, more accurate values of P^2 corresponding to the present $\frac{m_{00}^*}{m}$ values it is necessary to know the value of Δ_0 for this system. Here then Δ_0 has been taken to be 0.82eV for all the alloys since this is the accepted value for InSb⁹¹, while that for GaSb is very close to this value⁹⁸. Values of P^2 have been calculated corresponding to the smooth curve in fig. (5:12). This gives a value of about 21eV at InSb and 20eV at GaSb while again the values for the alloys

Specimen number	Comp x	I_1 ($\times 10^{-9} (\text{eV})^2 \text{m}$)	E_0^* (eV)	E_{Fo} (eV)	$\frac{m_{00}^*}{m}$
28	.160	.6491	0.244	0.1495	0.0151
29	.195	.6782	0.252	0.1577	0.0160
30	.290	.4606	0.282	0.1129	0.0197
31	.350	.4437	0.303	0.1045	0.0192
32	.400	.3147	0.322	0.0813	0.0242
33	.400	.4417	0.322	0.1056	0.0209
34	.470	.3201	0.355	0.0809	0.0246
35	.480	.3860	0.359	0.0926	0.0228
36	.500	.2774	0.368	0.0706	0.0254
37	.510	.2733	0.375	0.0687	0.0250
38	.530	.2826	0.382	0.0699	0.0245
39	.560	.2691	0.403	0.0674	0.0261
40	.600	.2332	0.427	0.0602	0.0288
41	.630	.1933	0.448	0.0484	0.0277
42	.730	.0972	0.523	0.0188	0.0326

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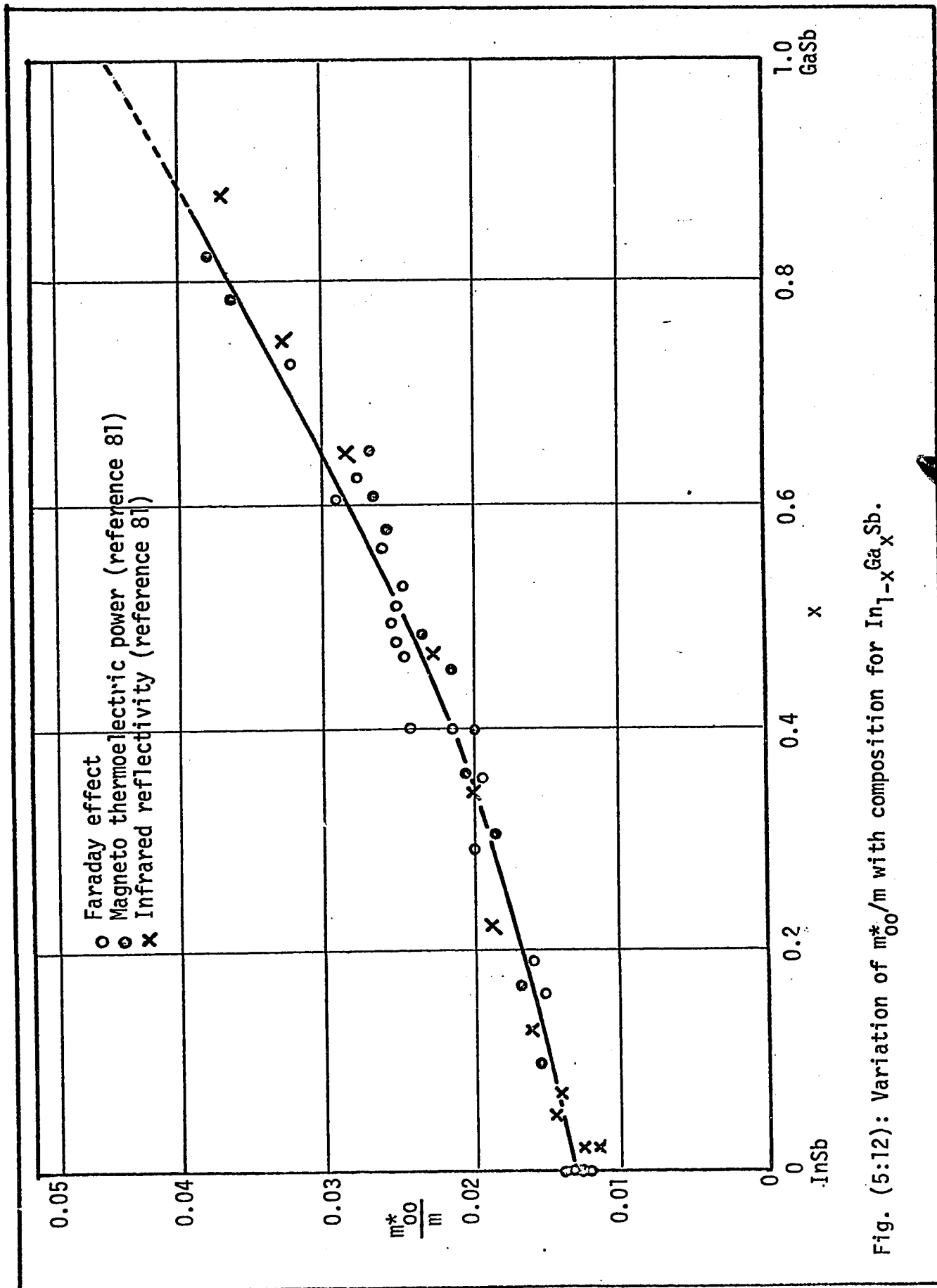


Fig. (5:12): Variation of m_{00}^*/m with composition for $\text{In}_{1-x}\text{Ga}_x\text{Sb}$.

show a shallow minimum at 19.4eV at $x = 0.6$. (See figure (5:11)).

At wavelengths where the absorption coefficient K is influenced by the presence of free carriers the relation between K and λ is given by⁹⁹

$$K = \frac{e^3}{4\pi^2 c^3 \epsilon_0 m^2 \eta} \frac{n_i}{(m_{ic}^*/m)^2 \mu_i} \lambda^2$$

where μ_i is known as the optical mobility of the free carriers. The absorption in a specimen at wavelengths away from the absorption edge can be described by

$$\log_{10} \left(\frac{I_0}{I} \right)_{Total} = \log_{10} \left(\frac{I_0}{I} \right)_{Free\ carriers} + \log_{10} \left(\frac{I_0}{I} \right)_{Background}$$

and if $I = I_0 \exp(-Kt)$

$$\log_{10} \left(\frac{I_0}{I} \right)_{Total} = \log_{10} \left(\frac{I_0}{I} \right)_{Background} + \log_{10} \left(\frac{1}{C} \right) + \frac{Kt}{2.303}$$

or

$$\log_{10} \left(\frac{I_0}{I} \right)_{Total} = Constant + \frac{e^3 (t/2.303)}{4\pi^2 c^3 \epsilon_0 m^2 \eta} \frac{n_i \lambda^2}{(m_{ic}^*/m)^2 \mu_i}$$

Hence the slope of the free carrier absorption is given by

$$S_3 = \frac{e^3(t/2.303)n_i}{4\pi^2 c^3 \epsilon_0 m^2 \eta (m_i^*/m)^2 \mu_i}$$

and on combining with equation [5:1] it can be seen that

$$\frac{S_1}{S_3} = 65.8 B \mu_i$$

and hence $\mu_i = \left(\frac{.01516}{B}\right) \frac{S_1}{S_3} \dots\dots\dots[5:20]$

Using [5:20] and the data in Tables 4J and 4K the optical mobility of some alloy specimen were calculated. The results are shown in Table 5G.

Specimen number	Composition (x)	Mobility cm ² /volt sec (μ_i)
28	0.16	9,600
29	0.195	6,700
30	0.290	15,300
31	0.350	9,840
32	0.400	4,300
33	0.400	5,000
35	0.480	5,000
36	0.500	4,100
37	0.510	6,500
38	0.530	6,100

T A B L E 5G

CHAPTER 6

C O N C L U S I O N S A N D D I S C U S S I O N S

i) Error Analysis

As seen before in Chapter 5 the two quantities from which the values of m_{00}^* are obtained are n_0 , the carrier concentration obtained from Hall effect measurements and the integral I_1 , which is obtained from the Faraday rotation measurements. For an error estimate in n_0 equation [3:3] and the definition for the Hall coefficient on page 82 are combined and hence

$$n_0 = IB/etV_H \dots\dots\dots[6:1]$$

$$(\Delta n_0/n_0) = (\Delta I/I) + (\Delta B/B) + (\Delta V_H/V_H) + (\Delta t/t) \dots\dots\dots[6:2]$$

In Chapter 3, section (v) it was pointed out that the Hall current was measured with a potentiometer set up and inaccuracies associated with this measurement are small. Similarly the Hall field and voltages were measured quite accurately. Specimen thicknesses were found to within 5 microns by taking a large number of measurements, generally about 16, over the surface of the specimen. In order to put numbers into [6:2] the data obtained on specimen 42 were chosen since here the observed Faraday rotation was small and these results will thus give an estimate of the maximum error. At a field of 3.198 w/m^2 and a current of 38.37 ma the Hall voltage was found to be 25.24 mV . Currents were read to $\pm 0.04 \text{ ma}$ and the voltages to $\pm 0.03 \text{ mV}$. Putting these values into [6:2] one gets

$$(\Delta n_0/n_0) = 0.1\% + 1.0\% + 0.1\% + 3.8\% = 5\%$$

and hence for specimen 42, $n_0 = (23.3 \pm 1.2) \times 10^{23} / \text{m}^3$.

Values for I_1 were found using equation [5:6] which gives

$$I_1 = \eta S_1 / D_1 B t \dots \dots \dots [6:3]$$

$$(\Delta I_1 / I_1) = (\Delta S_1 / S_1) + (\Delta B / B) + (\Delta t / t) \dots \dots \dots [6:4]$$

The error associated in η can be neglected in this analysis since corrections to η due to free carrier effects have been taken into account. The accuracy associated with the field measurement is taken from the manufacturer as being 1%. Errors in S_1 , the slope of the θ vs λ^2 curves are generated by errors in the measurement of θ only since the wavelengths are read to very high resolution. As has been mentioned in Chapter 3 section (iv) the θ values were found to within 0.5° . Sources of inaccuracy here are the misalignment of the analyser depolarization caused by the 45° mirrors, polarization caused by the source, mirrors and detector window and non-perfect polarization. If the accumulative error of 0.5° is superimposed onto the θ vs λ^2 graph for specimen 42 (p. 120) the error in the slope is seen to be $\pm 0.18 \times 10^{10} \text{ deg/m}^2$ and hence from [6:4]

$$\Delta I_1 / I_1 = 3.6\% + 1.0\% + 3.8\% = 8.4\%$$

and for this specimen $I_1 = (.0972 \pm .0080) \times 10^{-9} (\text{eV})^2 \text{m}$

In order to estimate the error in m_{00}^* four sets of (I_1, n_0) were fed into the computer for analysis as described in Chapter 5 section (ii)(c). These sets were (I_1^+, n_0^+) , (I_1^+, n_0^-) , (I_1^-, n_0^-) and (I_1^-, n_0^+) where the $\pm$ superscript indicates the addition or subtraction of the associated error. The following set of results were obtained for $(m_{00}^* / m, E_{F0})$.

$$(I_1, n_0) : (0.0326, 0.0188) \dots (I_1^+, n_0^+) : (0.0328, 0.0220) \dots (I_1^+, n_0^-) : (0.0302, 0.0203) \\ (I_1^-, n_0^-) : (0.0324, 0.0156) \dots (I_1^-, n_0^+) : (0.0350, 0.0173)$$

The maximum error in m_{00}^* is therefore ± 0.0024 and in E_{F0} , $.0032 \text{ eV}$.

ii) Summary of Results:

For GaSb, when a Kane model with parameters $m_{00}^*/m = 0.0447$ and $E_0^* = 0.771$ eV, was chosen to represent the (000) conduction band; it was found that for the $\langle 111 \rangle$ electrons $m_{1\tau}/m = 0.110$. The energy separation, ΔE , between the (000) and $\langle 111 \rangle$ minima was found to be 0.078 eV at 4.2°K. These values are in very good agreement with recent published results^{100,101}. At room temperature this energy separation was found to be 0.070 eV thus a very approximate temperature coefficient for this is -3.0×10^{-5} eV/°K. If a corrected value for ΔE at 77°K is used in the analysis of Liang et. al.⁴² the value of $m_{1\tau}/m$ obtained is close to that given above showing that the two sets of Faraday rotation data give very good agreement. Also the value of the scattering parameter, s , was found to be in the range $0.75 < s < 1.0$ for total carrier concentrations from 7×10^{17} to 4.0×10^{18} /cm³. This agrees very well with results of magneto-thermoelectric power measurements on similar material⁸¹. These measurements also allowed the energy separation, ΔE , to be investigated for each specimen. As in the case of InAs⁷⁸ and InSb¹⁰², it appears that for GaSb, ΔE is very sensitive to tellurium content in the sample. The value of $\frac{d}{dy} \Delta E = -0.5$ eV/atomic % Te would indicate that if more than 0.15 atomic % Te is added to GaSb at room temperature the $\langle 111 \rangle$ minima would be lower than the (000) minimum. There is some support for this in the optical absorption results for GaSb - Ga₂Te₃ alloys¹⁰³. In this case the addition of some 0.5 mole %

Ga_2Te_3 (i.e. 0.25 atomic % Te) caused the observed energy gap, E_g , to fall to 0.68eV. If this lower value of E_g is assumed to be a measure of the position of the $\langle 111 \rangle$ minima, which in pure GaSb is 0.80eV above the valence band maximum at room temperature, the change in energy of the $\langle 111 \rangle$ minima with tellurium content, y , is quite consistent with the value of $\frac{d}{dy} \Delta E$ given above. This would indicate that, in this case, the change in ΔE is caused by $\langle 111 \rangle$ minima moving towards the valence band, while for InAs it appeared that a corresponding change in ΔE was due to a movement of the (000) conduction band minimum from the valence band⁷⁸.

The variation of the bottom of the band effective mass with composition for the alloy specimens is in good agreement with that obtained by other independent measurements^{47,81}. If these results are compared with the results of Woolley and Thompson¹⁰⁴ the agreement is not good. In the latter work the effective mass for the alloys, was calculated using a more complicated band equation¹⁰⁵. Assumptions about the values of P^2 , Δ_0 (the spin-orbit splitting at Γ), and other energies involving the spacing between the valence band at Γ and higher bands, had to be made. P^2 was assumed to have a constant value of 23eV. A linear variation of Δ_0 (as in the present case) and of the higher band gaps was also assumed. The calculated results for the case of $\text{InSb}_{1-x}\text{As}_x$ gave much lower values for m_{00}^*/m than those obtained experimentally. For the $\text{In}_{1-x}\text{Ga}_x\text{Sb}$

system the discrepancy was not as large and here the calculated values of m_{00}^*/m for the alloys were slightly higher than the experimental values. If for the calculated values a Kane model of the form given in equation [2:36] is used the discrepancy is larger in both cases. To some extent the discrepancy is due to an incorrect choice of the various band gaps used in the calculations because of the fact that some of these have since been corrected from electroreflectance data, etc. However, it appears that the main error lay in the choice of $P^2 = 23\text{eV}$ for all values of x .

Further analysis on the variation of P^2 with alloy composition (fig.(5:11)) is now being undertaken by Vishnubhatla¹⁰⁹.

iii) Suggestions for future work:

Some of the results presented in this thesis have been arrived at by making assumptions which had some experimental evidence for basis. Although in some cases this evidence is rather scant these assumptions were seen to be not too drastic in the outcome of the results. There is, however, a great need for further work on both the compounds and the alloys. Now that low temperature optical facilities are available in this laboratory it is hoped that more work on the compound GaSb will be undertaken. For this compound, measurements of free carrier Faraday rotation together with magnetoresistance work at low temperatures would, it is hoped, justify some of the assumptions made here. The variation of m_{1x}/m with temperature and the variation of $\frac{d}{dy} \Delta E$ with temperature are two important required measurements.

For the $\text{In}_{1-x}\text{Ga}_x\text{Sb}$ system no values for m_{00}^*/m were given for $x > 0.80$. This is because in this range two band effects must be considered and on one specimen only the analysis becomes very complicated. On a number of specimens of different doping but the same composition, a solution can be found in this range.

In this thesis the effect of higher bands on the (000) conduction band model has only been briefly mentioned and perhaps a more rigorous analysis using the equation given by Cardona¹⁰⁵ will yield some interesting results.

The work presented here has been published in three separate papers which have been referred to as 76, 80, and 81.

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For the $\text{In}_{1-x}\text{Ga}_x\text{Sb}$ system no values for m_{00}^*/m were given for $x > 0.80$. This is because in this range two band effects must be considered and on one specimen only the analysis becomes very complicated. On a number of specimens of different doping but the same composition, a solution can be found in this range.

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APPENDIX (see page 131)

```

0001 DIMENSION CO(95),EF(95),EGS(95),EFMO(95),CONK(95),FEMO(95)
0002 DIMENSION AMSTAR(95),AI1(95),AI2(95)
      C CALCULATED EFFECTIVE MASS VALUES TO BE COMPARED WITH EXPERIMENT
      C THIS PROGRAM CALCULATES THE EFFECTIVE MASS OF (000) CONDUCTION
      C ELECTRONS USING A THEORY DEVELOPED BY PIDGEON AND SETS OF VALUES
      C OF THE EFFECTIVE MASS BAND GAP AND THE BOTTOM OF THE BAND
      C EFFECTIVE MASS... ENERGIES ARE MEASURED FROM THE BOTTOM OF THE
      C (000) CONDUCTION BAND.... ALL UNITS ARE IN THE M.K.S SYSTEM
      C READ(1,49) NSPEC,NMO
0003   49 FORMAT(2I3)
0004   READ(1,40)(CO(K),AMSTAR(K),CONK(K),EGS(K),EF(K),K=1,NSPEC)
0005   40 FORMAT(5E15.6)
0006   READ(1,44)(EFMO(L),L=1,NMO)
0007   44 FORMAT(F8.4)
0008   DO 125 L=1,NMO
0009   125 FEMO(L)=(1.0/EFMO(L))-1.00)
0010   AKT=0.02550
0011   ALPHA=3.8098E-20
0012   K=1
0013   105 L=1
0014   M=1
0015   N=1
0016   DELK=1.0000E+06
0017   WRITE(3,43) EF(K),EGS(K)
0018   43 FORMAT('1H1,14HFERMI ENERGY =,F7.4,10X,21HADJUSTED ENERGY GAP =,F6.
0019   14/)
0020   WRITE(3,42)
0021   42 FORMAT('1H0,2X,11HCOMPOSITION,24X,15HEFFECTIVE MASS ,5X,12HCARRIER
      1CONC,5X,15HEFFECTIVE MASS //)
0022   WRITE(3,41)
0023   41 FORMAT('1H ,4X,9H(PERCENT),23X,17HAT BOTTOM OF BAND,3X,14H(PER METE
      IR**3),7X,10H(CALCULATED//)
0024   102 EVEN1=0.000
0025   EVEN2=0.00
0026   ODD1=0.000
0027   ODD2=0.00
0028   AKE=1.0000E+06
0029   AKO=1.5000E+06
0030   DO 100 I=1,800
0031   AKE2=AKE*AKE
0032   AKO2=AKO*AKO
0033   VE=1.00+4.00*ALPHA*AKE2*FEMO(L)/EGS(K)
      VO=1.00+4.00*ALPHA*AKO2*FEMO(L)/EGS(K)
0034

```

APPENDIX cont'd.

```

0035 AE=SQRT(VE)
0036 AO=SQRT(VO)
0037 EE=(ALPHA*AKE2)-(0.50*EGS(K))+0.50*EGS(K)*AE
0038 EO=(ALPHA*AKO2)-(0.50*EGS(K))+0.50*EGS(K)*AO
0039 SE=(EE-EF(K))/AKT
0040 SO=(EO-EF(K))/AKT
0041 TE=EXP(SE)
0042 TO=EXP(SO)
0043 IF(M-1) 106,106,107
0044 106 BE=(AE+EFMO(L))/AE
0045      BO=(AO+EFMO(L))/AO
0046      UE=1.00/TE
0047      UO=1.00/TO
0048      HE=2.0+TE+UE
0049      HO=2.0+TO+UO
0050      F1E=((AKE**4)*(BE**3)/HE)
0051      F1O=((AKO**4)*(BE**3)/HO)
0052      EVEN1=EVEN1+F1E
0053      ODD1=ODD1+F1O
0054      107 IF(N-1) 108,108,109
0055      108 F2E=(AKE2/(1.00+TE))
0056      F2O=(AKO2/(1.00+TO))
0057      EVEN2=EVEN2+F2E
0058      ODD2=ODD2+F2O
0059      109 AKE=AKE+DELK
0060      100 AKO=AKO+DELK
0061      IF(M-2) 117,118,118
0062      117 A11(L)=(DELK/6.0)*(4.0*EVEN1+2.0*ODD1)*(ALPHA**3)*33.1053/AKT
0063      IF(A11(L)-AMSTAR(K)) 111,111,110
0064      111 M=2
0065      IF(L-2) 118,116,116
0066      110 CONTINUE
0067      118 IF(N-2) 115,124,124
0068      115 A12(L)=(DELK/6.0)*(4.0*EVEN2+2.0*ODD2)/(3.14159**2)
0069      IF(A12(L)-CONK(K)) 113,112,112
0070      112 N=2
0071      GO TO 119
0072      113 WRITE(3,50) CO(K),EFMO(L),A12(L),A11(L)
0073      50 FORMAT(1X,E12.4,27X,E12.4,5X,E12.4,8X,E12.4)
0074      IF(L-NMO)120,101,101
0075      120 L=L+1
0076      GO TO 102
0077      116 AMEFM=(EFMO(L)+(A11(L)-AMSTAR(K))*(EFMO(L)-EFMO(L-1))/(A11(L-1)-

```

APPENDIX cont'd.

```

0078      1A11(L)))
0079      GO TO 118
          119 CEFM=(EFMD(L)+(A12(L)-CONK(K))*(EFMD(L)-EFMD(L-1))/(A12(L-1)-
0080      1A12(L)))
          124 IF(M-2) 113,122,122
          122 WRITE(3,121) AMEFM,CEFM
          121 FORMAT(3X,4HEFFECTIVE MASS FOR EFFECTIVE MASS INTEGRAL =,E12.4,
0082      110X,4HEFFECTIVE MASS FOR CARRIER CONCENTRATION =,E12.4//)
          101 IF(K-NSPEC)103,104,104
          103 K=K+1
          GO TO 105
          104 STOP
0087      END

```

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COMPILER OPTIONS - NAME= MAIN,OPT=00,LINECNT=45,SOURCE,EBCDIC,NOLIST,NODECK,LOAD,MAP,NOEDIT,ID,N
ISN 0002 DIMENSION ETA(230),FOP5(230),FIP5(230),F2P5(230),F3P5(230)
ISN 0003 DIMENSION F2P0(230),FOP0(230),FIP0(230),F3P0(230)
ISN 0004 DIMENSION AN0(230),FUNC3(230)
ISN 0005 DIMENSION R(25),ALAMDA(25),THETA(25),ANI(230),FUNC4(230)
ISN 0006 READ(1,99)ETA(K),FOP5(K),FIP5(K),F2P5(K),F3P5(K),K=1,230)
ISN 0007 99 FORMAT(F10.4,4E14.7)
ISN 0008 READ(1,98)(FOP0(K),FIP0(K),F2P0(K),F3P0(K),K=1,230)
ISN 0009 98 FORMAT(10X,4E14.6)
ISN 0010 READ(1,1) NSPEC
ISN 0011 1 FORMAT(I3)
ISN 0012 AKT=0.0255
ISN 0013 CONS1=1.509E-11
ISN 0014 CONS2=8.963E-16
ISN 0015 CONS3=6.812E+27
ISN 0016 ALPHA=3.8098E-20
ISN 0017 PEFRAC=3.700
ISN 0018 DO 2 I=1,NSPEC
ISN 0019 READ(1,3) NDATA,ANOF,ANIF,AM00S,T,H,EGS
ISN 0020 3 FORMAT(I2,6E13.5)
ISN 0021 READ(1,4)(ALAMDA(J),THETA(J),J=1,NDATA)
ISN 0022 4 FORMAT(2E15.6)
ISN 0023 ES=EGS
ISN 0024 B=AKT/EGS
ISN 0025 M=1
ISN 0026 S=0.0
ISN 0027 28 K=1
ISN 0028 WRITE(3,200)
ISN 0029 200 FORMAT(1H1, 12H S 12H ANOF 12H AI1 12H
1 AI2 12H AI3 12H AI4 12H AMOS 12H
2 EF 12H R0 12H ANOR 12H ANOR1 //)
ISN 0030 L=1
ISN 0031 EF=-.100
ISN 0032 FEMO=((1.00/AM00S)-1.00)
ISN 0033 C1=16.7551*ALPHA**.5/(FEMO*FS)**1.5
ISN 0034 DELX=1.0E-03
ISN 0035 18 FVEN3=0.0
ISN 0036 EVEN4=0.0
ISN 0037 ODD3=0.0
ISN 0038 ODD4=0.0
ISN 0039 EVEN1=0.000
ISN 0040 FVEN2=0.00
ISN 0041 ODD1=0.000
ISN 0042 ODD2=0.00

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APPENDIX cont'd.

ISN 0043	XE=0.0	
ISN 0044	XO=0.5E-03	
ISN 0045	DO 100 IA=1,1000	
ISN 0046	SE=(XE-EF)/AKT	
ISN 0047	SO=(XO-EF)/AKT	
ISN 0048	IF(ABS(SE)-174.0)30,30,31	
ISN 0049	IF(ABS(SO)-174.0)32,32,31	
ISN 0050	30 IF(ABS(SE)-174.0)30,30,31	
ISN 0051	32 AE=EXP(SE)/(1.+EXP(SE))**2	
ISN 0052	AO=EXP(SO)/(1.+EXP(SO))**2	
ISN 0053	BE=XF*(XE+ES)	
ISN 0054	BO=XO*(XO+ES)	
ISN 0055	CE=2.0*XF+ES	
ISN 0056	CO=2.0*XO+ES	
ISN 0057	EE=ES/CE	
ISN 0058	EO=ES/CO	
ISN 0059	FE=1.0+FEMO*EE	
ISN 0060	FO=1.0+FFMO*EO	
ISN 0061	HE=1.0+FEMO*(EE**3)	
ISN 0062	HO=1.0+FEMO*(FO**3)	
ISN 0063	EVEN1=EVEN1+AE*BE**(2*S+1.5)*(FF**2)*HE*HE	
ISN 0064	ODD1=ODD1+AO*RO**(2*S+1.5)*(FO**2)*HO*HO	
ISN 0065	EVEN2=EVEN2+AF*BE**1.5	
ISN 0066	ODD2=ODD2+AO*RO**1.5	
ISN 0067	EVEN3=EVEN3+AE*BE**(S+1.5)*(FE*HE)	
ISN 0068	ODD3=ODD3+AO*RO**(S+1.5)*(FO*HO)	
ISN 0069	EVEN4=EVEN4+AE*BE**1.5*(FE**2)	
ISN 0070	ODD4=ODD4+AO*RO**1.5*(FO**2)	
ISN 0071	31 XE=XE+DELX	
ISN 0072	100 XO=XO+DELX	
ISN 0073	AI1=(DELX/6.0)*(4.0*EVEN1+2.0*ODD1)	
ISN 0074	AI2=(DELX/6.0)*(4.0*EVEN2+2.0*ODD2)	
ISN 0075	AI3=(DELX/6.0)*(4.0*EVEN3+2.0*ODD3)	
ISN 0076	AI4=(DELX/6.0)*(4.0*EVEN4+2.0*ODD4)	
ISN 0077	AI4=AI4*CI/AKT	
ISN 0078	ANOR=AI2/(AKT*3.14159**2*(ALPHA*ES*FEMO)**1.5)	
ISN 0079	AMOS=AMOS/(1.3888E+36*AI4)	
ISN 0080	P0=AI1*AI2/(AI3*AI4)	
ISN 0081	ANOR1=ANOR/RO	
ISN 0082	GO TO (24,25,26,39),L	
ISN 0083	24 IF(ANOF-ANOR1) 6,7,8	
ISN 0084	8 FF=EF+0.100	
ISN 0085	GO TO 18	
ISN 0086	6 FF=EF-0.010	

APPENDIX cont'd.

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ISN 0086      L=2
ISN 0087      GO TO 18
ISN 0088      25 IF(ANOF-ANOR1) 6,7,16
ISN 0089      16 EF=EF+.001
ISN 0090      L=3
ISN 0091      GO TO 18
ISN 0092      26 IF(ANOF-ANOR1) 17,7,16
ISN 0093      17 EF=EF-0.0001
ISN 0094      L=4
ISN 0095      GO TO 18
ISN 0096      39 IF(ANOF-ANOR1) 17,7,7
ISN 0097      7 CONTINUE
ISN 0098      WRITE(3,70)S,ANOF,A11,A12,A13,A14,AMOS,EF,RO,ANOR,ANOR1
ISN 0099      70 FORMAT(11E12.4)
ISN 0100      WRITE(3,102)
ISN 0101      102 FORMAT(1H,20X,12H  ETAL      ,12H  AN1R      ,12H  EF1      ,12H
1          DEL      ,12H  R1      ,12H  AN1F      ,12H  AM1T      //)
ISN 0102      SIZE=8.6
ISN 0103      F1=3.0*SIZE*(SIZE+2.0)/((2.0*SIZE+1.0)**2)
ISN 0104      AM1T=0.050
ISN 0105      23 K=1
ISN 0106      L=1
ISN 0107      15 GO TO (11,34,12,29),M
ISN 0108      11 FUNC2=F1*AN1F
ISN 0109      GO TO 35
ISN 0110      34 FUNC2=F1*AN1F*15.0*FOP5(K)*F1P5(K)/(16.0*F1P0(K)*F1P0(K))
ISN 0111      GO TO 35
ISN 0112      12 FUNC2=F1*AN1F*21.0*FOP5(K)*F2P5(K)/(25.0*F1P5(K)*F1P5(K))
ISN 0113      GO TO 35
ISN 0114      29 FUNC2=F1*AN1F*0.75*FOP5(K)*F3P5(K)/(F2P0(K)*F2P0(K))
ISN 0115      35 AN1(K)=4.0*CONS3*((AKT*AM1T)**1.5)*(SIZE**0.5)*FOP5(K)
ISN 0116      FUNC4(K)=FUNC2-AN1(K)
ISN 0117      GO TO (10,20),L
ISN 0118      10 IF(FUNC4(K)) 19,13,14
ISN 0119      14 K=K+10
ISN 0120      GO TO 15
ISN 0121      19 K=K-1
ISN 0122      L=2
ISN 0123      GO TO 15
ISN 0124      20 IF(FUNC4(K))19,13,13
ISN 0125      13 ETAL=(ETA(K)*FUNC4(K+1)-FUNC4(K)*ETA(K+1))/(FUNC4(K+1)-FUNC4(K))
ISN 0126      AN1R=AN1(K)+(ETAL-ETA(K))*(AN1(K+1)-AN1(K))/(ETA(K+1)-ETA(K))
ISN 0127      EF1=ETAL*AKT

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APPENDIX cont'd.

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ISN 0128 DEL=EF-FF1
ISN 0129 P1=ANIR/(ANIF*F1)
ISN 0130 SUM1=0.00
ISN 0131 SUM2=0.00
ISN 0132 SUM3=0.00
ISN 0133 SUM4=0.00
ISN 0134 SUM5=0.00
ISN 0135 AMIF=(AMIT*3.0*SIZE)/((1.0+2.0*SIZE)*F1)
ISN 0136 DO 5 J=1,NDATA
ISN 0137 P(J)=SORT(REFRAC*PEFRAC-CONS2*ANOF*ALAMDA(J)*ALAMDA(J))*{(R0+R1)*ANIF
1*AMOS/(ANOF*AMIF))/AMOS)
SUM1=SUM1+P(J)*THETA(J)*ALAMDA(J)*ALAMDA(J)
SUM2=SUM2+P(J)
SUM3=SUM3+P(J)*R(J)*THETA(J)/(ALAMDA(J)*ALAMDA(J))
SUM4=SUM4+P(J)*R(J)/(ALAMDA(J)**4)
SUM5=SUM5+ALAMDA(J)**4
5 CONTINUE
COEF=(SUM1*SUM4-SUM2*SUM3)/(SUM5*SUM4-SUM2*SUM2)
PART1=ANIF*AMOS*AMOS*R1*CONS1*H*T
PART2=COEF*AMOS*AMOS
PART3=R0*CONS1*ANOF*I*H
CHECK=PART2-PART3
IF(CHECK)38,38,37
37 AMIG=SORT(PART1/(PART2-PART3))
IF(AMIG -AMIF)21,21,22
22 AMIT=AMIT+0.001
GO TO 23
21 WRITE(3,95) ETAL,ANIR,EF1,DEL,R1,ANIF,AMIT
95 FORMAT(20X,7E12.4)
WRITE(3,91),P1,AMIG
9 FORMAT(1H,3X,16HSPECIMEN NUMBER,12,3X,18HSCATTERING FACTOR=,F6.2
1,3X,36HBOTTOM OF (111) BAND EFFECTIVE MASS=,F6.3/)
38 IF(M-4.0)27,2,2
27 M=M+1
S=S+.5
GO TO 28
2 CONTINUE
STOP
END
ISN 0158
ISN 0159
ISN 0160
ISN 0161
ISN 0162
ISN 0163
ISN 0164

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