SHUBNIKOV-DE HAAS EFFECT UNDER UNIAXIAL STRESS:

A NEW METHOD FOR DETERMINING DEFORMATION POTENTIALS AND
BAND STRUCTURE INFORMATION IN SEMICONDUCTORS

DISSERTATION

Presented to the Graduate Council of the
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By

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The problem with which this investigation is concerned is that of demonstrating the applicability of a particular theory and technique to two materials of different band structure, InSb and HgSe, and in doing so, determining the deformation potentials of these materials. The theory used in this investigation predicts an inversion-asymmetry splitting and an anisotropy of the Fermi surface under uniaxial stress. No previous studies have ever verified the existence of an anisotropy of the Fermi surface of semiconductors under stress. In this work evidence will be given which demonstrates this anisotropy. Although the inversion-asymmetry splitting parameter has been determined for some materials, no value has ever been reported for InSb. The methods presented in this paper allow a value of the splitting parameter to be determined for InSb.
The theory used in this work was developed to describe the variation of the energy spectrum of a material under deformation. This theory is generally applicable to semiconductors of the zinc blende structure. In this theory the spin-orbit split band is neglected and a 6x6 Hamiltonian is constructed, the elements of which depend in a complicated manner upon the energy band parameters, deformation potentials, and the applied strain. Diagonalization of the Hamiltonian gives six eigenvalues, the largest two of which are the conduction band eigenvalues needed for defining the Fermi surfaces. Constant energy contours of the two split conduction bands can then be calculated, and integration gives the extremal cross-sectional areas which are directly related to the SdH frequencies. Thus, at each stress value the frequencies can be determined. From the fractional frequency changes the deformation potentials may be calculated. In addition a beat frequency is calculated from the two frequencies which can be used to determine the splitting parameter of InSb.

In this investigation the Subnikov-de Haas effect has been used to study band structure changes in InSb and HgSe. The samples of HgSe studied had electron concentrations ranging
from $8 \times 10^{16}$ to $4 \times 10^{18}$ cm$^{-3}$. The variation in carrier concentrations was accomplished by annealing the samples in either Se or Hg Vapor. The InSb studied had a concentration of $2 \times 10^{17}$ cm$^{-3}$. Silver paste was applied around the ends of the sample for current contacts and platinum wire spring probes were used for the Hall and resistivity voltages. The stress was always applied along the current direction. All SdH measurements were made using magnetic field modulation and phase sensitive detection techniques.

From this investigation values of the deformation potentials in InSb were found to be $b = -1.7 \pm 0.2$ eV, $d = -1.9 \pm 0.4$ eV, and $C_2 = -1.7 \pm 0.3$ eV; in HgSe, $d = -2.7 \pm 0.4$ eV, $b = -1.2 \pm 0.2$ to $-1.6 \pm 0.3$ eV depending upon concentration. From the experimental data the value of the splitting parameter $B_3$ was found to be $-3.3 \pm 0.5 \hbar^2/2m_0$. This value of $B_3$ is consistent with $B_3$ values for other materials. In addition to the determination of the above values, the anisotropy of the Fermi surface in semiconductors under uniaxial stress was experimentally established for the first time. Although previous theoretical work had shown that the conduction band should become anisotropic under
application of uniaxial stress, until the present time, no experimental proof for this anisotropy had been given.
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CHAPTER I

INTRODUCTION

In the first section of the introduction the material, mercury selenide, and its properties are discussed. After description of the compound, background information on important studies pertinent to this investigation will be outlined. A large portion of this discussion will be devoted to establishing the generally accepted band structure of mercury selenide. In the second section an introduction to stress related experiments and its effects will be presented. Primary emphasis will be on uniaxial stress and the effect it has on a material such as mercury selenide. In the final section the objectives and importance of this investigation will be presented.

Background Information on Mercury Selenide

Mercury Selenide, HgSe, is a compound formed with an element from group-II in the periodic table, mercury, Hg, and an element from group-VI, selenium, Se. This compound
has a cubic, zinc-blende crystal structure. The zinc-blende lattice results from replacing the two group-IV atoms of the diamond lattice basis with one group-II and one group-VI atom. Thus, HgSe lattice structure has no inversion center. Physically, mercury selenide is a very brittle, metallic material with a grayish color. An abbreviated table of the properties of HgSe is given in Table I. For a more complete description of these properties see Neuberger.¹

Very little was known about the band structure of the mercury chalcogenides until the last decade. In the past ten years or so rapid progress has been made in developing experimental techniques for obtaining information about the electronic structure of materials. Thus, since 1960 the mercury chalcogenides have been widely investigated. Mercury telluride is undoubtedly the most extensively investigated material because of its practical application for infra-red detectors. Any properties found in HgTe would suggest like characteristics in HgSe due to their similarity. Thus some of the important properties of HgTe will be discussed in this section. Both HgSe and HgTe have small bandgaps and high mobility. However, only
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<td>Formula</td>
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<td>Molecular Weight</td>
<td>279.51</td>
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<tr>
<td>Density</td>
<td>7.95</td>
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<td>2.25</td>
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<td>cubic, zincblende</td>
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<td>Space Group</td>
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<tr>
<td>Lattice Parameters</td>
<td>6.0854 ± 0.0002</td>
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<tr>
<td></td>
<td>2.633</td>
<td></td>
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<tr>
<td>Phase Transition</td>
<td>7.5 Kbars</td>
<td>15 Kbars</td>
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<td>Melting Point</td>
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<tr>
<td>Sublimation Temperature</td>
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<tr>
<td>Specific Heat</td>
<td>4.7</td>
<td>10⁻²cal/g°C</td>
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<td>Debye Temperature</td>
<td>137.2</td>
<td>°K</td>
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<tr>
<td></td>
<td>151</td>
<td>°K</td>
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<td>Thermal Conductivity</td>
<td>0.016</td>
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<td>Thermal Coefficient of Expansion</td>
<td>30°C 500°C</td>
<td>10⁻⁶°C⁻¹</td>
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<tr>
<td></td>
<td>-7</td>
<td>1.8</td>
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<td>Elastic Constants (Stiffness)</td>
<td>0°C</td>
<td>10¹¹ dynes/cm²</td>
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<tr>
<td></td>
<td>C₁₁</td>
<td>6.900</td>
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<tr>
<td></td>
<td>C₁₂</td>
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<td></td>
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<td>Compressibility</td>
<td>1.753</td>
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<td>$10^{-3}$-$10^{-4}$</td>
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<td>Mobility</td>
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<td>Electron</td>
<td>12,000 to 40,000</td>
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<td>Effective Mass</td>
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<td>Electron</td>
<td>0.045 ± 0.003</td>
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<tr>
<td>Hole</td>
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<td>$m_o$</td>
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<td>Energy Gap,</td>
<td>Eg -0.24</td>
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<td></td>
<td>Et -0.07</td>
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<td>-4.6 ± 0.2</td>
<td>$10^{14}$eV/K</td>
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<td>$10^5$cm/sec</td>
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n-type HgSe has been produced while both n- and p-type HgTe have been grown. Crystals of HgSe are typically grown by the Bridgeman method, and once the crystals are grown their concentration may be varied by annealing the samples. The annealing process will be discussed in a later chapter.

After a brief introduction to the material itself, next some of the investigations that have been performed on HgSe are considered. Electrical properties of mercury selenide were initially measured on pressed powder specimens. In addition the thermal magneto-resistive effect and the Nernst coefficient were also measured on samples of this type. With the development of techniques for growing single crystals, a variety of electrical, optical, and mechanical properties were investigated. A study of angular dependence of the magnetoresistance in HgSe led Harman to the conclusion that the conduction band is nearly spherically symmetric and centered at the origin in k-space. Similar measurements by Gobrecht et al. also confirmed the spherical conduction band. Oscillatory magnetoresistance data obtained by Whitsett gave effective mass data that was in agreement with the reflectivity and
magnetoreflectivity data of Wright et al.\textsuperscript{14} The results of Wright et al.\textsuperscript{14} and Whitsett\textsuperscript{9} were in quantitative agreement with a nonparabolic conduction band model proposed by Kane\textsuperscript{15} for indium antimonide. Thus, the conduction band in mercury selenide was indicated to be a nonparabolic, spherically symmetric band.

In an earlier work where a parabolic band was used in the analysis of the data by Harman\textsuperscript{16}, the scattering mechanism for the charge carriers was suggested to be due to acoustical phonons. This conclusion was upheld by the work of Tsidilkovskii\textsuperscript{4} and Rodot and Rodot.\textsuperscript{17} However, in a later work, Harman\textsuperscript{18} re-interpreted the data in terms of Kane's band model and concluded that due to optical phonons, polar scattering predominates in HgSe. In addition, Harman and Strauss\textsuperscript{8} used Kane's model in the interpretation of Hall coefficient versus temperature data. This Hall coefficient versus temperature data for HgSe was analyzed on the assumptions of one nonparabolic conduction band, one parabolic valence band, and exact Fermi-Dirac statistics. This analysis gave a thermal energy gap, $E_t$, for HgSe of approximately $-0.07$ ev.\textsuperscript{8}
In this same investigation, optical absorption coefficient data as a function of wavelength supported the semimetal model for HgSe. The conduction band parameters used in the above analysis were obtained from optical and electrical measurements on high electron mobility samples of HgSe. The negative energy separation between the conduction and valence bands led to the conclusion that mercury selenide was a semimetal. This particular analysis showed that the E(k) calculated by Kane for InSb could apply quantitatively to HgSe and yielded an energy gap at \( k = 0 \) of approximately 0.1 to 0.2 ev. at room temperature. Very recently work by Broerman has shown that the overlap energy is much smaller, perhaps only 0.001 to 0.01 ev.

Later studies on the Hall coefficient and resistivity data of HgTe (recall HgSe is very similar to HgTe) gave an intrinsic carrier concentration much too high to be consistent with a positive thermal energy separation, \( E_t \). Thus, it was concluded that HgTe was also a semimetal. Therefore, HgSe as well as HgTe was suggested to have a higher-lying valence band at \( k = 0 \). However, the origin of this higher-lying valence band was a mystery, since the
band did not appear to fit the band structure pattern for zinc-blende compounds. Normally, zinc-blende III-V compounds have one light electron ($\Gamma_6$) conduction band separated by an energy gap, $E_g$, at $k = 0$ from an almost mirror image light hole ($\Gamma_8$) valence band and a heavy hole ($\Gamma_8$) valence band. There existed three possibilities for the explanation of the structure in HgSe.

One possibility for the higher-lying valence band was that an entirely new band independent of the bands from the $\Gamma_6$ and $\Gamma_8$ states was coming into the picture. Another explanation was that the heavy hole band, which came from one to the $\Gamma_8$ states, was bent up by a few tenths of an electron volt. Assuming that either of these possible explanations was true would have been a strong departure from the band structure of other zinc-blende materials. The third possibility suggested inverted ordering of the $\Gamma_6$ and $\Gamma_8$ states. This was suggested by Groves and Paul after they had shown that the gray tin band order was inverted. This inverted energy ordering was applied to HgTe by Harman et al. This band model was found to be consistent with both the III-V and II-VI compounds with zinc-blende structure.
This inverted band model has been established for HgTe and HgSe by different types of experiments. Peotrzkowski, et al.\textsuperscript{24} have analyzed thermoelectric power versus hydrostatic pressure data on HgTe to determine the ordering of the $\Gamma_6$ and $\Gamma_8$ states. Oscillatory magnetoresistance data taken by Stradling and Antcliffe\textsuperscript{25} gave further evidence of the inverted band structure of HgTe. Groves, et al.\textsuperscript{26} added additional evidence through interband magnetoreflection studies on HgTe. Although the results do not establish the ordering in HgSe, De Meis, et al.\textsuperscript{27} have measured the pressure dependence of the absorption edge in doped HgSe which suggests the inverted ordering. In addition, using the band parameters obtained by Whitsett from Shubnikov-de Haas measurements, Broerma\textsuperscript{19} has shown that the mobility versus electron concentration data are in agreement with calculations utilizing a $\Gamma_8$ band instead of a $\Gamma_6$ band. These results give additional evidence for the inverted band structure of mercury selenide. Galazka, et al.\textsuperscript{28} have developed analytical expressions which relate Shubnikov-de Haas frequency to warping of the $k=0$ conduction band. Shubnikov-de Haas frequency versus concentration data was used to unambiguously
conclude that the conduction band in HgSe has $\Gamma_8$ symmetry. Therefore, unlike many zinc-blende materials, HgSe, as well as HgTe, has a conduction band of $\Gamma_8$ symmetry lying higher than the $\Gamma_6$ band. The conduction and valence bands are also degenerate at the zone center or $k=0$. A schematic inverted energy band model for HgSe is shown in Fig. 1. The $\Gamma_8$ valence band and the $\Gamma_8$ conduction band at $k=0$ are separated from the $\Gamma_6$ valence band by the energy gap, $E_g$. The spin-orbit split band, $\Gamma_7$, lies an amount $\Delta$ below the conduction band.

Unlike the diamond lattice, which requires $E(k)$ to be two-fold degenerate for all $k$, the zinc-blende lattice has no inversion symmetry. If the zinc-blende material has a finite spin-orbit splitting, $E(k)$ will no longer be two-fold degenerate at all $k$. The existence of an inversion-asymmetry splitting has been predicted for some time\textsuperscript{29}. This splitting is due to a combination of spin-orbit interaction and antisymmetric potential associated with dissimilar basis atoms of the zinc-blende structure. However, the effect was small and difficult to observe experimentally. Whitset\textsuperscript{9} originally concluded that beating
Fig. 1--Inverted Band Structure Proposed for HgSe
effects seen in SdH oscillations were due to an almost spherical Fermi surface with slight bulges in the [111] directions. Later, using Whitsett's Shubnikov-de Haas data containing the beating patterns, Roth concluded from a quantum-mechanical theory that the beats seen in the oscillatory magnetoresistance of HgSe are due to inversion-asymmetry splitting. On the other hand, Seiler et al. have analyzed beating patterns in the SdH oscillations in terms of a semiclassical model of two Fermi surfaces split by inversion asymmetry. However, certain features of the beating effects cannot be fully explained by this semiclassical model. In addition the semiclassical model gives a splitting factor of about one-half that of the quantum-mechanical model. Additional information on the mercury compounds may be obtained from several review articles.

Effects of Uniaxial Stress

Before proceeding with a discussion of methods to obtain more information on HgSe, some background on stress related investigations is necessary. In general, the
physical properties of a solid depend on its mechanical state of strain. In particular, the electrical resistivity may be a function of the state of strain in a material. The change of the resistivity of a solid with the application of strain or stress was discovered several years ago and was known as the elastoresistance or piezoresistance effect. For certain solids this effect is quite large. Since stress and strain are related through the elastic compliance tensor, these two effects are also directly related. In a material with known elastic constants, knowledge of one effect implies knowledge of the other. These effects can be interpreted in terms of electronic band structure parameters and can be very useful in studying various features of the band structure of a solid. There are two types of stress which can be conveniently applied to a solid: hydrostatic pressure and uniaxial tension or compression. Techniques which allow various measurements on materials under these types of stress have been described in the literature. Subjecting a sample to hydrostatic pressure does not change the crystal symmetry. (This statement does not apply to the case in which high pressure can
cause a transformation to different crystal structure.) Therefore, in many cases the effects produced on galvanomagnetic measurements by hydrostatic pressure are comparatively simple.

On the other hand the effect of uniaxial stress can yield some very striking results. During the past decade uniaxial stress has become a powerful tool in the investigation of the properties of semiconductors. Generally, the application of uniaxial stress to a semiconductor changes its symmetry and thus removes or modifies any degeneracies associated with that symmetry. Changes occurring in the symmetry can be detected by investigating the electrical properties of the semiconductor. Often extrapolation of stress data to the zero stress condition can yield valuable information about the properties of the undeformed material. Some information yielded by stress measurements are the following: the location of band extrema, effective masses, lattice dynamical properties, deformation potentials, and symmetries of interband optical transitions. The concept of deformation potentials has been found to be useful in the theory of lattice scattering.40

Following the deformation potential concept, consider a uniaxial, compressive stress applied along a [100] or
[111] crystallographic axis of a semiconductor having a zinc-blende crystal structure. The four-fold degenerate $E_8$ bands are split into two doubly degenerate states (as shown in Fig. 2) with $M_j = \frac{3}{2}$ and $M_j = \frac{1}{2}$. The $M_j = \frac{1}{2}$ state (light-hole band) moves up in energy relative to the $M_j = \frac{3}{2}$ state (heavy-hole band). Thus, the $E$ versus $k$ relations may vary with stress. The changes with uniaxial stress that occur in the $E$ versus $k$ relations can be described by the deformation potentials $a$, $b$, $C_1$, and $d$ which were introduced by Bir and Pikus. The number of deformation potentials needed to describe changes in a material may vary depending on the symmetry involved. In cubic materials, for transitions between $p$-like and $s$-like bands, only three valence band deformation potentials are needed to describe the behavior of the $k = 0$ gap. However, in a material of lower symmetry, such as a hexagonal one, six coefficients are necessary to describe the effect of stress on the band edge.

Now let us define the quantities $a$, $b$, $C_1$, and $d$. The hydrostatic-pressure deformation potential, $a$, describes the shift of the center of gravity of the valence band,
while b and d are uniaxial-stress deformation potentials for strains along the crystallographic directions, [100] and [111], respectively. In addition, C₁, is the conduction-band deformation potential. For example, the bottom of the conduction band is shifted up for a compressive stress by an amount C₁e, where e is the trace of the strain tensor (this is exactly true for [100] stress and a very good approximation for other stress directions.) Now, the hydrostatic deformation potential of the direct energy gap is a+C₁. Therefore, the energy gap will change by an amount \((a+C₁)(S₁₁+2S₁₂)X\) where \(S₁₁\) and \(S₁₂\) were elements of the elastic compliance tensor. For uniaxial, compressive stress \(X=−\sigma\) where \(\sigma\) is the magnitude of the stress. Finally, consider an example demonstrating b and d. When stress is applied along a [100] direction the valence bands split by an amount, \(2\sqrt{3}b|S₁₁−S₁₂|X\). Similarly, for stress along a [111] direction, the bands split by an amount \(1/\sqrt{3}|d|S₄₄X\).

Objectives of this Investigation

This investigation was undertaken to determine the applicability of a particular theory for InSb type semiconductors
of the material HgSe, and in doing so determine the deformation potentials, b and d. The values of the deformation potentials in HgSe have not previously been obtained. Once the theory is developed, its usefulness will be demonstrated by applying this same theory in InSb (a more well-known material). Analytical expressions are shown to give results consistent with a computer program that was developed to perform calculations using the above mentioned theory.

The theory used in this study predicts an inversion-asymmetry splitting and an anisotropy of the conduction band under uniaxial stress. The inversion-asymmetry splitting parameter has been measured for some materials but not for InSb. In this investigation an attempt will be made to obtain the splitting parameter for both InSb and HgSe. In addition an attempt will be made to demonstrate the anisotropy of the conduction band in semiconductors under application of uniaxial stress. Although it has been theoretically predicted for some time, no direct experimental proof for this anisotropy has ever been given.

The remainder of this thesis is separated in five chapters. Chapter II presents the theory of the effect of
Fig. 2 - E(k) Curves in Unstressed and Stressed HgSe
deformation on the energy spectrum which eventually allows
determination of the deformation potentials, b and d.
In Chapter III the techniques and equipment used in gathering data for this study are discussed. Then, in Chapter IV the theory is applied to data collected on InSb. From a fit of the theory to data the deformation potentials and splitting parameter are determined. Chapter V contains data from numerous samples of HgSe over a wide concentration range. Following the procedure outlined in Chapter IV deformation potentials are obtained for HgSe. Finally, Chapter VI contains the conclusions of this investigation.
CHAPTER II

THEORY

A theory for the variation of the energy spectrum of a material with deformation has been developed by Bir and Pikus (42). This theory is applicable to semiconductors of the InSb type, that is, zinc blende structure. With the application of stress a material's symmetry may change, thus affecting any degeneracies involved. This can result in a change of the energy band structure and thus change the galvanomagnetic properties of the sample. In this study, the theory of Bir and Pikus has been used to determine the effects of strain on the energy band structure of mercury selenide. In the succeeding pages, the theory and assumptions relevant to this investigation will be discussed.

In determining the effect of uniaxial deformation on the energy band structure of zinc blende semiconductors, Bir and Pikus constructed a Hamiltonian by using Luttinger's (44) representation of the basis functions. Taking into account the strong interaction between the s- and p-bands, they constructed a matrix simultaneously for
both bands. That matrix is as follows:

\[
\begin{pmatrix}
\lambda & 0 & 0 & i/\sqrt{3}K_+ & \sqrt{2/3}K_z & iK_- \\
0 & \lambda & K_+ & -i\sqrt{2/3}K_z & 1/\sqrt{3}K_- & 0 \\
0 & K^* & F' & H' & I' & 0 \\
-i/\sqrt{3}K^*_+ & i/\sqrt{3}K^*_z & H'^* & G' & 0 & I' \\
\sqrt{2/3}K^*_z & 1/\sqrt{3}K^*_z & I'^* & 0 & G' & -H'^* \\
-iK^*_z & 0 & 0 & I'^* & -H'^* & F' \\
\end{pmatrix}
\]

where

\[
\begin{align*}
\lambda &= E_g + B_1 k^2 + c_1 e, \\
K_+ &= iB_2 k_1 + B_3 k_1 + k_1^2 + c_2 e_{i1+i1, i+2}, \\
K^* &= 1/\sqrt{2} (K_x + iK_y), \\
F' &= 1/2 (L'+M') (k_x^2 + k_y^2) + M' k_z^2 + 1/2 (\ell+m)(e_{xx}^1 + e_{yy}^1) + me_{zz}, \\
H' &= -i/\sqrt{3} [N' (k_x k_z - ik_y k_z) + n(e_{xz} - ie_{yz})], \\
I' &= (1/2/3) [(L'-M') (k_x^2 - k_y^2) - 2iN' k_x k_y + (\ell - m)(e_{xx} - e_{yy}) - 2ie_{xy}], \\
G' &= 1/3 F' + 2/3 [M' (k_x^2 + k_y^2) + L' k_z^2 + m(e_{xx} + e_{yy}) + \ell e_{zz}].
\end{align*}
\]

In this simplified Hamiltonian, \(E_g\) is the energy gap when there is no deformation, \(e\) is the trace of the strain tensor \((e = e_{xx} + e_{yy} + e_{zz})\), \(B_1\) is a constant of interaction between the conduction band and all \(\Gamma_15\) symmetry bands other than the top valence bands, \(B_2\) is the momentum matrix element.
(P = -\(\frac{i\hbar}{m_0}\) < S |P_x |X>), and B_3 is a constant giving the amount of inversion-asymmetry splitting of the bands. In materials which have inversion symmetry B_3 is zero.

The parameter C_1 is the conduction band deformation potential, while C_2 is a constant which relates the strain interaction between the conduction and valence bands.

Next, in order to define the parameters l, m, and n one needs first to define the strain perturbation operator, \(D_{ij}\). This strain operator is defined as

\[
D_{ij} = \frac{h^2}{m_0} \sum_{i,j} \left( \frac{\partial^2}{\partial x_i x_j} + \frac{m_0}{h} V_{ij}\right)
\]

where

\[
V_{ij} = \frac{V(r')}{\delta_{ij}} \bigg|_{e=0}
\]

and V(r') is the crystal potential in the deformed lattice. Now, the matrix elements l, m, and n are then defined as

l = <X |D_{XX} |X>, m = <X |D_{YY} |X>, n = 2 <X |D_{XY} |Y>, where the wave functions, |x> and |y>, have the angular symmetry of the atomic p-functions. Interactions between the s- and p-bands were not taken into account in these coefficients because such interactions would only result in corrections on the order of \(e^2\) and \(ek^2\).
Next, L', M', and N' are higher band parameters similar to those used by Dresselhaus, et al (42). However, these parameters, as with l, m, n, do not include the interaction between the s- and p-bands, while the parameters of Dresselhaus do take this interaction into account. Up to this point, the deformation potentials have not been mentioned in the theory. They are included in the terms l, m, n through the following expressions:

\[ a = \frac{1}{3} (l+2m), \quad b = \frac{1}{3} (l-m), \quad d = \frac{n}{\sqrt{3}}. \]

Therefore, the deformation potentials are contained in the matrix expression and ultimately will be in the \( E(e,k) \) relations.

With most of the parameters being defined, consider next the approximation used in this theory. First, the authors have neglected terms containing \( ek \) and \( ek^2 \) due to their smallness as compared to other terms. Also, for similar reasons in terms on the order of \( B_3^2 \) only those independent of k and 3 have been considered. In addition in HgSe \( E_g < 2 \Delta (E = -0.22 \text{ eV}, \Delta = 0.45 \text{eV}) \) where \( \Delta \) is the spin-orbit coupling parameter. Consequently, the spin-orbit split band has been neglected in this theory.
Now, from the matrix, D, the secular equation \(|D-E| = 0\) has the form:

\[
((\lambda - E)[E^2 - E(G' + F') + G'F' - |I'|^2 - |H'|^2]) + 2/3K^2E + \phi)^2 - |\theta|^2 = 0
\]

where the function \(\theta\) describes the splitting of the band proportional to \(k^3\) or \(k^3E\). The exact analytical expression for \(\theta\) is extremely complicated involving many individual terms. Several days were spent solving for \(\theta\) and \(\phi\) without any further approximations. These parameters were so involved that little if any utility could be seen in carrying the analytical solutions to their logical end. This was especially true, since the numerical results were of primary interest. Therefore, in theory one could solve the secular equation given above for six values of \(E\), but in practice it is much more rewarding to diagonalize the 6th order matrix and obtain the energy eigenvalues by computer techniques. Hence, the effect of deformation on the spectrum is obtained.

At this point the energy values can be determined for various stress values at a given \(k\). If the correct coordinate system has been chosen, this \(k\) value will lie perpendicular to the magnetic field. This being desirable,
a transformation of coordinates was performed initially such that \( \vec{B} \) is always parallel to one of the new coordinate axes, and where \( K \) and \( \phi \) are a set of polar coordinates lying in the plane perpendicular to the magnetic field \( B \). In addition, the polar angle \( \theta \) will be between the field direction and a crystallographic direction lying in the plane of rotation of the magnetic field. (The details of this transformation are given in Appendix B). With the coordinate system described above, \( \phi \) may be systematically varied \( k \) values corresponding to the Fermi energy can be determined. From these values numerical integration yield the cross-sectional area of the Fermi surface perpendicular to the magnetic field.

The cross-sectional area of the Fermi surface is directly related to the frequency or period of the Shubnikov-de Haas oscillations. (A detailed discussion of the Shubnikov-de Haas effect may be found in many of the new texts on solid state physics, therefore only a brief discussion will be given in this section). In many materials, such as HgSe, some of the physical
parameters show a variation with magnetic field which is periodic in the reciprocal of the field strength. This group of phenomena is associated with the quantized motion of the charge carriers in the magnetic field. When a magnetic field is applied to a free-electron system, the charge carriers motion in a plane perpendicular to the field becomes quantized. Therefore, the quasicontinuous distribution of energy levels in the conduction band is broken into degenerate Landau level subbands. The energy separation between the minima of adjacent Landau levels is equal to $W_c'$, where $W_c$ is cyclotron-resonance frequency, and the $n$th Landau level lies at $(n + 1/2) / W_c'$ above the zero-field point, where $n$ takes on positive integer values including zero. Next, as the magnetic field increases, the energy separation between Landau levels becomes larger also. This increase results in the successive passing of these levels through the Fermi level. As a result, oscillations will occur in the transport properties of the material. In our case, the magnetoresistance varies in such a manner. Since Shubnikov and de-Haas (45) were the first to observe an oscillatory magnetoresistance,
such a phenomena is termed the Subnikov-de Haas effect.

The period of SdH oscillations is related to the extremal cross-sectional area of the Fermi surface by the following expression (46):

$$ P = \frac{2 \pi e}{c \hbar A_f} $$

where the units are expressed in the MKS system. Therefore, using this relation a theoretical period or frequency may be calculated for the already calculated areas previously discussed.

The computer program developed to perform the calculations discussed in this section is given in Appendix C. This program finds the eigenvalues of the matrix, calculated the cross-sectional area of the Fermi surface, and determines the Shubnikov-de Haas frequencies. In addition the cross sections of the Fermi surface may be mapped from this program output. All of the above operations may be carried out for any magnetic field direction perpendicular to the stress direction and the stress direction may be along a [100], [111], or [110] crystallographic axis.
CHAPTER III

EXPERIMENTAL TECHNIQUES

Sample Preparation

The material used in this study was prepared by Robert Galaska (47), using the Bridgeman method. A double distillation technique under vacuum was used to remove any gaseous contaminants and the tube was sealed. The quartz capsule containing the compound was then placed in a furnace and the growth run was started. The resulting ingot contained single crystal regions from which samples were cut by means of an electrical discharge machine. The single crystals were oriented by x-ray diffraction techniques, using a Norelco X-ray unit equipped with a Laue back-reflection camera. The individual samples were then cut with a Servomet spark machine using a 5 mil tantalum wire as the cutting tool. Typical sample dimensions were 7-9x1.1 x 1.1mm. Samples of parallelepiped shapes were cut having either the [100], [110], or [111] direction along the long dimension of the crystal.
At this point the samples were polished, using 1000-grit silicon carbide grinding powder, distilled water, and a flat glass plate. This procedure produced extremely parallel sides. Considerable attention was given to the problem of obtaining parallel surfaces. This was especially true on the faces to which the force was applied in order to assure uniform distribution of the stress and to prevent unwanted torques. Following the mechanical polishing, the samples were etched in a bromine (1 part) and methanol (20 parts) solution for approximately one and a half to two minutes and then rinsed in methanol. Sample orientation was rechecked by X-ray techniques before subjecting the samples to final annealing. Annealing capsules were made from 7 mm. O.D. glass tubing. A sample, along with either Se or Hg (high purity), was placed in a capsule which was then evacuated to between $10^{-5}$ and $10^{-6}$ mm. of Hg and sealed off under vacuum. The general procedure was to anneal the sample in a Se or Hg rich atmosphere at a given temperature and pressure for a given length of time (48).

The capsule was placed in a cavity bored in a two-inch diameter copper bar, and the bar was placed in a
furnace. Although the furnace was very accurately controlled for temperature, the copper bar assured even better temperature stability and homogeneity. Temperatures from 50°C to 300°C and times from 1 day to 21 days were used. The lower temperatures (50-100°C) and longer times (14-21 days) were used with the Hg saturated capsules, while the Se saturated capsules were annealed at higher temperatures for shorter time periods. Carrier concentrations obtained by this procedure ranged from \(7 \times 10^{16}\) to \(6 \times 10^{18}\) cm\(^{-3}\). The Hg filled capsule yielded higher carrier concentrations than the Se filled capsules.

After the samples were annealed, the crystals were removed from the annealing capsule and again etched in a bromine and methyl alcohol solution (1 to 30) and rinsed in methyl alcohol. Next the samples were measured and checked for any visible defects with a Unitron depthscope. The crystals were then ready to be mounted in the stress apparatus.

**Stress Apparatus**

The basic principle of the stress apparatus is the balance or lever arm concept. The operation of the device
is illustrated in the cut-away drawing shown in Fig. 3. Uniaxial compression is achieved by exerting an upward force on the pulling frame A, which is attached to the lower end of the pulling rod C. The support tubing B connects the apparatus to the sample holder. The upper end of the pulling rod is connected by means of a steel wire D to the left end of the lever arm H which is pivoted by the support F attached to the top of the aluminum housing of the apparatus. A stainless steel pin is fixed in the lever arm and each of its ends rest in the precision ball bearings G which are light-pressed in each side of the support. The right end of the lever arm is connected to a force transducer J by means of a small chain I, which is also attached to a pin which rests in another precision ball bearing G. This transducer can be raised or lowered by means of the screw and rotating shaft arrangement K, shown in greater detail in Fig. 4. Mounted on the bottom of the shaft is the gear L turned by a variable-speed gear motor M. Counterbalance weights E can be adjusted so that the lever arm is balanced prior to the sample being mounted. The ends of the chamber housing the lever arm are sealed with plexiglas flanges N for visual inspection of the
Fig. 3--Cut-away Drawing of the Uniaxial Stress Apparatus.
Fig. 4--Screw and Rotating Shaft Arrangement for Providing Force to Lever Arm.
lever arm position. For variable temperature runs, a calorimeter is attached which encloses the support tubing and pulling frame.

Figure 4 shows a cut-away illustration of the screw and rotating shaft arrangement which is used to raise and lower the force transducer. The load-bearing probe is connected to the lever arm by the small chain. The transducer is mounted on a fine-threaded shaft which has a keyway cut in it. This shaft is screwed into a cylinder which is free to rotate inside a fixed casing. Rotation of the cylinder is accomplished by means of a shaft attached to the cylinder and extending into the external atmosphere through a vacuum-tight O-ring seal. A gear attached to the end of this shaft is rotated by a smaller gear mounted on the shaft of a reversible, variable-speed motor so that the application of stress on the sample is slow and smooth. The gears have a 10-to-1 ratio and the motor has 0-to-1 rpm speed range.

The force transducer is a Daytronic Model 152 A-10 linear variable differential transformer (LVDT) which produces an output voltage proportional to the applied force. This voltage is fed to a Model 300-D Daytronic
Transducer Amplifier-Indicator with Type 71 High Sensitivity Differential Transformer Input Module. Once the system is calibrated, the applied force on the sample can be read directly from the indicator panel meter. Calibration of the stress apparatus prior to the experiments was accomplished by attaching known kilogram weights (accurate to 0.5%) to the pulling frame and noting the scale reading on the indicator panel meter. A maximum of 35 kg was applied during calibration of the transducer. The magnitude of the stress can then be determined from the meter reading of the force and the cross-sectional area of the sample.

The sample holder, shown in detail in Figs. 5 and 6, is primarily made of a non-magnetic Be-Cu alloy. Its design is similar to that reported by Balslev (49). The sample is mounted between the two pistons as shown in Fig. 5. Brass cups are mounted in teflon cups, which provide electrical isolation for the sample, and they are in turn mounted in the pistons. The ends of the sample are mounted in small recessions in the brass cups. The position of the upper piston is fixed in the cylinder by a stainless steel pin, but the lower piston is free to
Fig. 5--Internal Parts of Sample Holder.
HEATER COIL
PHENOLIC BLOCK
ACCESS TO SAMPLE
Be-Cu CYLINDER
OPTIONAL LOCATION OF SPRING CONTACTS
LOWER PISTON

S. S. PULLING ROD
S. S. SUPPORT TUBE
PULLING FRAME

Fig. 6--External Parts of Sample Holder.
move up and down with the pulling frame. The pistons were precisionly machined so that each had two narrow belts which have slightly larger diameters. This was done to minimize the contact area between the pistons and the cylinder wall and thereby reduce the frictional drag on the pistons. In addition, these belts and the inner wall of the cylinder were highly polished with very fine grinding powder.

Because of difficulty in soldering signal probes to HgSe, two phenolic blocks were attached to the outside of the cylinder as shown in Fig. 6. These were used as bases for spring-contact signal probes. Even on materials that are easily soldered, stress can produce a breakdown of probe contacts. Thus spring contacts are useful in many instances, and they do not interfere with the operation of the pulling frame. However, some problems may be encountered with spring contacts. This type of probe is more sensitive to mechanical vibration and generally introduces more noise to the signals. In addition to the two phenolic blocks, two coils of #30 Evanohm wire were wound around the cylinder to act as heaters. When the heaters are in use, a stainless steel can is placed around the pulling frame and support tube.
This "inner cryostat" may be evacuated or filled with helium gas to form a heat leak from the sample holder to the cooling bath. With the appropriate cooling bath, temperatures from about 1° to 300°K, may be obtained. The heaters were calibrated with a CryoCal precision thermometer. Reproducability of low temperatures less than 300°K, were found to be within 1%.

The particular construction of this stress apparatus has several advantages. When the apparatus is mounted on the low temperature cryostat, the lever arm and transducer chamber is common with the low temperature chamber, thus avoiding the friction involved in passing a pulling rod through a vacuum-tight drive gear on the transducer assembly. Any friction at this point does not interfere with the calibration or operation of the apparatus. Also, with the larger support tubing being under compression and the small inner pulling rod being under tension, the dimensions of the two are such that the heat flux to the lower parts of the cryostat is very small (49). If the inner rod had been used for compression, it would have had to be much thicker to support the compressions without bending. This would have considerably increased heat flow to the sample holder.
Cryogenic System

A schematic of the cryogenic and vacuum system is shown in Fig. 7. The stress apparatus sits atop a double-dewar system with the sample holder extending into a liquid helium bath. In order to obtain a temperature of less than 4.2°K, a vacuum was pumped on the stress apparatus and dewar with a Kinney large-capacity vacuum pump. The pressure was maintained by adjustment of a large ball valve and a small needle valve in parallel. The pressure above the helium was measured with mechanical gauges and an oil manometer. The pressure reading was converted to temperature by the use of the "1958 He Scale of Temperatures." For temperatures above 4.2°K and less than 30°K, the heater coils and calorimeter can discussed in the previous section were used.

Magnetic Fields

A Pacific Electric Motor Company electromagnet was used throughout this experiment. The magnet was a model 12A-LI with 6-inch diameter pole caps and a 1 3/4 inch air gap. Magnetic fields of up to 24.0 kilogauss with 1x10^-5 homogeneity were obtainable in the region of the sample.
Controlling the electromagnet was a Varian Associates Fieldial power supply (Model V-Fr 2701) which was field regulated. This power supply was able to sweep the magnetic field linearly between pre-set time limits. In this experiment a voltage proportional to the field was fed to the x-axis of an X-Y recorder (EAI Model 1130). This voltage was provided by a Bell Hall-Pak (Model B H-701) mounted on one of the magnet pole faces. This current for the Hall probe was supplied by a constant current source constructed in the physics department electronics shop.

In addition to the dc magnetic field just described a small ac magnetic field was also used. This ac field was superimposed on the dc field and produced ac signals in the sample which were detected by ac instrumentation. The ac magnetic field was produced by a coil wound around one of the pole caps. This modulation coil was powered by a power amplifier (McIntosh Model MG 275) which was driven sinusoidally by a Hewlett-Packard 200 CD audio oscillator. The peak-to-peak value of the ac modulation field was dependent upon the dc field value and also upon the modulation frequency. These points are discussed
in detail by Alsup (50). With a 43-Hz frequency the modulation coil was capable of producing a magnetic field of approximately 200 gauss peak-to-peak throughout the dc magnetic field range. In this work all data were taken using a 43 Hz frequency.

Detection Equipment

The standard dc potentiometric circuit was used in measuring the Hall coefficient and the zero field resistivity. This circuit is shown in a block diagram in Fig. 8. Voltages between sample contacts or across the 1 ohm standard resistor were measured with a millivolt potentiometer (Leeds and Northrup K-3) using a Keithley microvolt-ammeter (Model 150B) as a null detector. The current for the sample was supplied by a constant current source (Hewlett-Packard Model 6177B). Most data were taken using approximately 40 milliamps current, although 100 milliamps were used with a few of the higher conductivity samples. Potential changes on the order of 0.5 microvolts were readily detectable. The Hall measurements were made with both +I and -I, as well as +H and -H. Averaging of the four voltages was done to eliminate any thermoelectric or misalignment signals.
Fig. 8—D. C. Measurement Equipment.
During an ac measurement, the circuitry shown in Fig. 9 was used. The sample shown in this figure sits in liquid helium inside the double dewer system previously discussed. The applied ac modulation field, also discussed in an earlier section, produces an ac voltage across the sample. This signal is then amplified and fed to a PAR HR-8 lock-in amplifier which selects a given frequency and rectifies it by a conventional phase-sensitive detection method. The dc signal produced by the lock-in amplifier then goes to the y-axis input of an X-Y recorder.

As the dc magnetic field is increased, the sample resistance increases monotonically. The signal produced by the ac modulation field is proportional to the rate at which the resistance changes with field. Oscillations superimposed on the increasing resistance create corresponding fluctuations in the slope and hence in the signal. Therefore, as the dc magnetic field is swept to higher field values, the quantum oscillations of the magneto-resistance amplitude-modulate the carrier signal produced by the modulation field. The ac detection equipment demodulates the carrier signal, producing a slowly varying...
Fig. 9—A. C. Measurement Equipment.
dc output as a function of magnetic field. Thus, a plot of this dc output versus the Hall probe voltage on an X-Y recorder exhibits the desired Shubnikov-de Haas oscillations.

The same constant current supply used in the dc measurements was used for the ac measurements. In general the same current ranges were also used, 40 to 100 milliamps. The current was transmitted to the sample via one pair of a six conductor cable made from individually twisted pairs of wire. The remaining two pairs were for the Hall and resistivity signals. The signal passed through an electrolytic capacitor to avoid saturation of the preamplifier by the dc component of the sample signal. A PAR (Princeton Applied Research) type-B preamplifier with a gain of 350 was used at all times. From the preamp the signal entered a PAR HR-8 lock-in amplifier. This phase sensitive detector (lock-in amplifier) selected the desired frequency and phase and fed a rectified signal to the X-Y recorder.

The data in this investigation were taken using a modulation field frequency of 43 Hz and a reference frequency of 86 Hz. This was done for two reasons. First,
the quantum oscillations are superimposed on a monotonically increasing resistance which does not increase linearly with magnetic field. The second harmonic is second derivative like, and gives a more constant base line for the oscillations. Secondly, detection at the second harmonic gives more enhancement to the low field relative to the high field oscillations. In order to have the modulation field at one frequency and to detect at twice this frequency while maintaining a constant phase relation, it is necessary to create harmonics in the reference channel of the lock-in amplifier. The harmonics were created by a combination of diodes and resistors, half-wave rectifier, as described in the PAR lock-in amplifier manual. The narrow-bandpass input amplifier of the lock-in is tuned to the desired harmonic. The fundamental frequency (43 Hz) chosen was high enough to prevent ripples from occurring on the Hall probe magnetic field sensor, was low enough to avoid any heating problems, and was not a sub-harmonic of 60 Hz.
CHAPTER IV

VERIFICATION OF THEORY

Since the deformation potentials of HgSe had never been determined, a well-known material, indium antimonide, was chosen as a test for the theory used in this investigation. In this chapter the results of our studies on InSb are reported. In addition to determining the deformation potentials in InSb, the first direct experimental evidence for the inversion-asymmetry splitting of the conduction band is also reported.

The SdH measurements were carried out on a sample of n-type InSb having an electron concentration of $\sim 2 \times 10^{17}$ cm$^{-3}$. Changes in the SdH frequency were observed when the magnetic field direction was transverse to the stress direction, $\sigma || [110]$. These data were determined by measuring the shift in magnetic field position of a point of constant phase in the SdH oscillations as a function of stress. Data exhibiting the frequency shift are shown in Fig. 10. There is no indication that the phase of the SdH oscillations is changing with stress; only the period
Fig. 10—83H Oscillations at Different Stresses in InSb with \(n=2\times10^{17}\) cm\(^{-3}\).
or frequency of the oscillations changes. The phase is also found to be constant with stress in bismuth$^{52}$ and, as seen later in this paper, in HgSe. At zero stress the SdH frequency, $F$, exhibits an anisotropy with respect to magnetic field direction which is characteristic of a warped Fermi surface,$^{53}$ $F(\bar{1}11) > F(\bar{1}\bar{1}0) > F(001)$. The theoretical work of Bir and Pikus$^{42}$ showed that the conduction band of InSb type semiconductors should become anisotropic under application of uniaxial stress. However, (until the present time) no direct experimental proof of a Fermi surface anisotropy induced by stress has been given for any semiconductor. In this study unambiguous evidence is presented that the conduction band of InSb becomes anisotropic with the application of uniaxial stress. Under application of a stress of about 1 kilobar or greater along the [110] crystallographic direction, the anisotropy changes such that $F(\bar{1}1\bar{0}) > F(\bar{1}\bar{1}1) > F(001)$.

Figure 11 shows a plot of frequency versus magnetic field direction for a stress of 0 and 2 kilobars. This particular anisotropy under stress is the result of the originally almost spherical Fermi surface changing into a general ellipsoid with principal axes along [110], [1\bar{1}0], and [001]
Fig. 11—Frequency versus Magnetic Field Direction in Unstressed and Stressed InSb.
directions. Figure 12 shows the extremal cross sections of the Fermi surface for the magnetic field along three major directions and at two different stress values. These cross sections were calculated by the method described in Chapter II. At zero stress, the two constant-energy contours are similar to those reported for HgSe, but with a much smaller band splitting. The energy contour then changes shape under applied stress. Comparison of the figures with and without stress indicates the Fermi surface is changing to a distorted ellipsoid.

Earlier studies of n-type InSb have shown no indications of beating effects, even though the theoretical existence of the inversion-asymmetry splitting is well known. Previously, a beat frequency in the SdH oscillations has only been seen in the semiconductors HgSe and GaSb. The studies on these materials enabled values of the inversion-asymmetry splitting of the conduction band to be estimated. In this investigation beating effects were observed in the SdH oscillations of InSb for the first time. By comparing the beating effect data with the E versus k theory containing the effects of
Fig. 12—Extremal Cross Sections of InSb Fermi Surfaces with and without Stress.
uniaxial stress, the first values of the inversion-asymmetry splitting for the conduction band in InSb are determined.

The determination of the deformation potentials $b$, $d$, $C_2$, and the band splitting parameter, $B_3$, is broken up into two parts. This separation is facilitated by the fact that the calculated frequency changes are not affected by the value of $B_3$, as expected; the value of $B_3$ does, of course, affect the beating effects. In addition, the calculated beat frequency depends very little upon $d$ and $b$. Thus, in the first part values of $B_3$ and $C_2$ will be estimated. In order to accomplish this a model must be chosen. Before discussing the model, values of the band parameter used in the calculations will be given. In all computations $E_g = 0.235$ eV, $P = 9.0 \times 10^8$ eV-em, and higher band parameters $B_1 = 0$, $L' = -2.6$, $N' = -4.3$, in units of $h^2/2m_0$. A value of $(a+C_1) = -7.0$ was chosen for the calculations used in this investigation. In practice the value effects the calculations only slightly. For example, changing $(a+C_1)$ from -7.0 to -6.0 only causes $\sim 0.1\%$ change in the computed results discussed later.

A simple semiclassical model of two Fermi surfaces split by inversion asymmetry is used in the interpretation.
The cross sections of the extremal areas, and hence a difference frequency, \((F_1 - F_2)\), are calculated from the constant energy contours obtained from the Bir and Pikus theory described in Chapter II. In the simplest beating effects model, the nodal position is given by the term \(\cos\left(\pi(F_1 - F_2)/B\right)\).

Figure 13 shows data which illustrate the emergence of the beating effects for \(B\parallel[001]\) as compressive uniaxial stress is applied along a [110] crystallographic direction. Beating effects are also observable for \(B\parallel[1\overline{1}1]\) but at higher stress values than for \(B\parallel[001]\). No beating effects could be observed up to 4 kilobars for \(B\parallel[1\overline{1}0]\).

Since only one nodal position for a given magnetic field direction is ever observed under stress, the difference frequency cannot be directly measured. However, the simple beat model implies that the value of the first nodal position is given by \(B_0 = 2(F_1 - F_2)\), which is directly observable. Figure 14 shows a plot of the observed nodal positions as a function of stress for \(B\parallel[001]\) and \(B\parallel[1\overline{1}1]\). The nodal positions vary almost linearly with stress in the range where they are seen.

A striking thing about the stress data above 1 1/2 kilobar is that the highest field nodal position is observed
Fig. 13--Emergence of Beat in SdH data of InSb for B||[001].
for \( B \parallel [001] \), rather than \( B \parallel [1\overline{1}1] \). In \( \text{HgSe} \)\(^9,13,30,63\) and \( \text{GaSb} \)\(^64,65\) at zero stress, the first nodal position for \( B \parallel [1\overline{1}1] \) is always observed at a higher magnetic field than for \( B \parallel [001] \). (As seen in the next chapter this remains true with application of stress to \( \text{HgSe} \).) In Fig. 14 the solid and dashed lines represent the theoretical variation of \( 2(F_1-F_2) \) with stress for \( B \parallel [001] \) and \( B \parallel [1\overline{1}1] \), respectively. Note that at zero stress, the computed nodal position for \( B \parallel [1\overline{1}1] \) is higher than for \( B \parallel [001] \), in agreement with the \( \text{HgSe} \) and \( \text{GaSb} \) data. Because of the small value of \( B_0 \), beats have not previously been seen in \( \text{InSb} \), and in this study they were only observable above \( 1 \frac{1}{4} \) kilobars. For this reason experimental verification of the beat position at zero stress is lacking. In fitting the data to the theory, the best fit by eye judgment gives \( B_3 = -3.3^{+0.5}_{-1.0} \frac{\hbar^2}{2m_0} \) and \( C_2 = -1.7^{+0.3}_{-0.5} \text{eV} \). As can be seen in Fig. 14, a detailed quantitative fit is not necessary since only a qualitative fit of the model to the data is reasonable. Recall, the quantity \( C_2 \) is the deformation potential which takes into account the stress-induced coupling between the valence and conduction bands for materials, like \( \text{InSb} \), which do not have inversion symmetry. Since the splitting parameter, \( B_3 \), has not been
Fig. 14--Beat Nodal Position versus Stress for $B \parallel \langle 001 \rangle$ and $B \parallel \langle 1\bar{1}\bar{1} \rangle$. 
determined previously for InSb, only comparison to other materials can be made. In GaSb, a quantum mechanical model was used to estimate a value of \( |B_3| = 9.6 \hbar^2/2m_e \).

Using a classical model to interpret the same data gives a value of \( |B_3| = 4.8 \hbar^2/2m_e \). A semiclassical model of two Fermi surfaces split by inversion asymmetry was also used in the analysis of beating effects in HgSe to obtain a value of \( |B_3| = 3.45 \hbar^2/2m_e \). The quantum-mechanical model gave \( |B_3| = 6.5 \hbar^2/2m_e \) for HgSe. In a recent study on the effect of uniaxial stress on the magnetophonon effect in InSb, \( |C_2| \) was estimated to be \( 1 \pm 1 \) eV. Thus, the values of \( B_3 \) and \( C_2 \) determined in this investigation are consistent with other measurements.

With the values of \( B_3 \) and \( C_2 \) determined, values of \( b \) and \( d \), valence-band deformation potentials, were then estimated from a fit of the theory to data presented in Fig. 15. The solid lines represent the theoretical curves for \( b = 1.7 \pm 0.2 \) eV and \( d = -1.9 \pm 0.4 \) eV as obtained from the computer program given in appendix C. From piezoemission studies, \( b = -2.0 \pm 0.15 \) eV and \( d = -5.0 \pm 0.5 \) eV; from magnetoreflection experiments, \( b = -2.0 \) eV and \( d = -4.9 \) eV; from piezobirefringence measurements.
Fig. 15--Changes in SdH Frequencies versus Stress InSb, \( n = 2 \times 10^{17} \text{cm}^{-3} \).
b = 1.8 eV and d = -6.4 eV; from magnetophonon studies, b = -2.0 ± 0.2 eV and d = -5.0 ± 0.2 eV. The value of b is in good agreement with the above values, but the value of d is much smaller. The reason for this difference in the d values is not yet understood.

In order to check the computer program, analytical expressions were derived that when compared to experimental data give b and d values. This was particularly desirable since there was some discrepancy in the d value as obtained from computer techniques. In Appendix D the change in Fermi energy with stress, as well as analytical expressions for the cross-sectional areas of the Fermi surfaces, are calculated. A Fermi level change was included in all the calculations that determined the parameters previously discussed. A plot of the Fermi level versus stress for three different concentrations is given in Fig. 16. The Fermi energy as a function of stress may be written \( E_f^S = E_f^0 (1 + \alpha \sigma) \), where \( \alpha \) is given by the appropriate quantities from Appendix D. Numerically, \( \alpha = -1.45 \times 10^{-11} \) for a value of \( (a + C_1) = -7.0 \). Following the procedure outlined in Appendix D yields an analytical expression for the frequency
Fig. 16--Fermi Energy Versus Stress for Three InSb Concentrations, $2 \times 10^{18}$, $2 \times 10^{17}$, $2 \times 10^{16}$ cm$^{-3}$ respectively from top to bottom.
changes in terms of $b$ and other known parameters. Comparison of this expression (Eq. D-16) to experimental data gives a value of $b = -1.7 \pm 0.1 \text{ eV}$. Next, using the data shown in Fig. 17 (the ratio of $F_{110}/F_{001}$), a relation between $b$ and $d$ may be obtained, Eq. D-20. Using this relation and the previously determined $b$ value, a value of $d = -2.1 \pm 0.4 \text{ eV}$ is obtained. Thus, from analytical expressions the data gives a value for $b$ and $d$ which is in very good agreement with the computer program values. Therefore, the theory gives good results for $b$ and a $d$ value that is smaller than expected.
Fig. 17--Ratio of SdH Frequency when B||[1\bar{1}0] to the Frequency when B||[100] versus Stress.
CHAPTER V

EXPERIMENTAL DATA AND RESULTS

This section will be broken into four sub-sections. The first sub-section will discuss frequency antisotropy with respect to magnetic field direction and the tendency of this anisotropy to become ellipsoidal-like under stress. Under the second sub-heading the changes in frequency with stress for major crystallographic directions, as well as the concentration dependence of the frequency changes, will be presented. From this data the deformation potentials, $b$ and $d$, will be extracted. The third section discusses the orientation of the sample by use of the beating effects. The angular dependence of the beats with and without stress are presented. Then in the final section some of the aspects of the beating effects under application of uniaxial stress are presented and discussed.

Ellipsoidal Nature Under Stress

It is important to establish the orientation of the crystal being studied. In practice there are three methods
by which the orientation of the samples can be determined. First, the method used during sample preparation, is the Laue x-ray technique. This technique is only useful before the sample is mounted in the stress apparatus. Once the crystal is placed in the apparatus and prepared for an experimental run, two other methods remain available for determining orientation in the plane perpendicular to the stress direction. The easiest and principal method used in this investigation (angular dependence of the beating effects) will be discussed in a later section. At present the variation of frequency with magnetic field direction is of interest. Therefore, next consider the importance of this frequency anisotropy in determining the crystal's orientation in the plane of the magnetic field. The following discussion will refer to a crystal with a [110] stress direction. The period or frequency with respect to magnetic field direction at zero stress has been presented by Galaska, et al. From these data it can be seen that a plot of the frequency anisotropy will allow verification of the crystallographic directions which lie in the magnetic-field plane. While the frequency anisotropy is useful in determining orientation at zero stress, its major usefulness in this study is to demonstrate
the ellipsoidal nature of the Fermi surface under stress. Therefore, let us next consider the nature of the Fermi surface under stress.

At zero stress the SdH frequency, $F$, exhibits an anisotropy with respect to magnetic field direction which is characteristic of a warped Fermi surface, $^{53} F(\{1\bar{1}\}) > F(\{\bar{1}0\}) > F(001)$. Under application of uniaxial stress, changes occur in the SdH frequency. These changes are dependent upon the magnetic field direction as well as the concentration of the material. Figures 18a, 18b, and 18c show SdH oscillation data for different stress values with the magnetic field parallel to a [001], [1\bar{1}1], and [1\bar{1}0] direction, respectively. From the oscillatory data the frequency can be determined. Figs. 18a, b, c were taken with a crystal of concentration $3.1 \times 10^{17}$ cm$^{-3}$. Upon examination of this data, one finds the largest frequency shift with stress occurring for $B \parallel [001]$ and the least change in frequency when $B \parallel [\bar{1}0\bar{1}]$. Therefore, since the frequency change is different for different magnetic field directions, the frequency anisotropy is changing. Figure 19 displays this anisotropy in HgSe when the stress value is one kilobar. Galaska, et al.$^{28}$ present zero stress in a previous investigation. The circles in Fig. 19
Fig. 18a--SdH Frequency at Different Stress Values for Sample #3 with $B \parallel [001]$. 
Fig. 18b—SQUID frequency at different stress values for sample #3 with B || [III].
Fig. 18c—Saw frequency at different stress values for sample #3 with $B_{\parallel \left[110\right]}$. 

Detector Response

$B_{\parallel \left[110\right]}$

$\sigma = \frac{3}{4}$  $\sigma = \frac{1}{2}$  $\sigma = \frac{1}{4}$  $\sigma = 0$

$B (kG)$

1  2  3  4  5
Fig. 19--Frequency Anisotropy at 1 kilobar for Sample #7; Circles are Experimental Data, Solid Line Represents Theoretical Ellipsoidal Model.
represent experimental data while the solid line represents a theoretical ellipsoidal model as can be obtained from Appendix D. Comparison of Fig. 19 and the zero stress data indicate a definite change toward an ellipsoidal-type anisotropy, that is, $F(1\overline{1}0) > F(1\overline{1}1) > F(001)$.

Before proceeding further, the question of a phase shift in the SdH Frequency with stress needs to be considered. As previously stated in Chapter IV no phase shift with stress is seen in the SdH oscillations of bismuth$^{52}$ and InSb. Figure 20 shows a plot of $1/B$ versus $N$ for sample #1 in a stressed and unstressed state. Since the two curves have the same intercept, no phase change with stress is indicated to occur in the SdH oscillations of HgSe. Now, let us return to the frequency changes observed in HgSe.

As previously mentioned, the changes in the SdH frequency with stress depend upon the concentration of the sample. Figure 21 shows data from a sample of concentration about $8 \times 10^{16}$ cm$^{-3}$. Note that there is a much larger shift in peak position with stress then in Fig. 18a. Thus, the magnitude of the frequency shift increased with a decrease in the concentration of the sample. Although the magnitude of the frequency changes with stress are dependent upon the
Fig. 20--Reciprocal Magnetic Field versus Number of Periods for Sample #1.
Fig. 21--SdH Frequency at Different Stress Values for Sample #1.
number of carriers, the frequency anisotropy changes to ellipsoidal form for each sample of different concentration. Figure 22 shows results similar to Fig. 19 but for a sample of lower concentration (about $8 \times 10^{16} \text{cm}^{-3}$). It is apparent in both cases that the frequency anisotropy is becoming more ellipsoidal. Therefore, the ellipsoidal nature of the Fermi surface under uniaxial stress appears to be true for all concentrations of HgSe. As stated in Chapter IV, theoretical work indicated that the Fermi surface in InSb type semiconductors should become anisotropic under uniaxial stress, but until now no experimental proof for this anisotropy has been given. In Chapter IV this anisotropy was demonstrated for InSb and in this section it has been shown to exist for HgSe.

**SdH Frequency Changes**

SdH data, as well as other electrical measurements, were collected on numerous HgSe crystals over a wide concentration range. The results of Hall and resistivity measurements at zero stress are tabulated in Table II for several samples. Of primary interest in this investigation was the frequency changes that occur in the SdH oscillations.
Fig. 22--Frequency Anisotropy at 1 kilobar for Sample #1; Circles are Experimental Data, Solid Line Represents Theoretical Ellipsoidal Model.
<table>
<thead>
<tr>
<th>Sample Number</th>
<th>( n = \frac{1}{R_H e} ) (10^{17} \text{ cm}^{-3})</th>
<th>( \rho ) (10^{-4} \text{ ohm-cm})</th>
<th>( \mu_H = \frac{R_H}{\rho} ) (10^{4} \text{ cm}^2/\text{V-sec})</th>
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</tr>
<tr>
<td>10</td>
<td>49.0</td>
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<td></td>
</tr>
</tbody>
</table>

From SdH period data \( n = 3.1 \times 10^{17} \text{ cm}^{-3} \)
under uniaxial stress. Already some SdH period with stress data has been presented in the previous section. In this section the frequency shifts with stress for the major crystallographic directions and the concentration dependence of these changes are investigated. Ultimately, the deformation potentials, b and d, will be determined from the fractional changes in the SdH frequencies with stress.

In Fig. 21, SdH oscillations for sample #1 (the lowest concentration investigated) are shown. Fractional changes in the SdH frequency are determined by measuring the shift in magnetic field positions of the resistance minima or maxima shift to lower fields as the stress increases. This implies that the frequency of the oscillations is decreasing with stress, since the phase of the oscillations is unchanged by the stress. Sample #1 had ~10.2% per kilobar change in frequency for B||[001]. The fractional changes in the SdH frequency when the magnetic field direction is transverse to the stress direction, σ||[110], are shown in Fig. 23 for B||[001], B||[111], and B||[110]. The solid lines represent the best-fit theoretical predictions.

The data from sample #1 are explained by the general theory of Bir and Pikus outlined in Chapter II and
Fig. 23--Fractional changes in SdH Frequency versus Stress for Sample #1; Solid Lines Represent Theoretical Predictions.
demonstrated in Chapter IV. As with InSb, the Fermi energy in HgSe is expected to depend upon stress,\textsuperscript{42} and for this analysis it is assumed that the Fermi energy changes linearly with stress as $E^S_f(\sigma) = E^O_f(1+\alpha\sigma)$. This is the same functional form of the stress dependence of the Fermi energy as used with InSb in the previous chapter. For InSb, an analytical expression gives $\alpha = -0.0145 \text{ kbar}^{-1}$ while the best-fit computer program gives $\alpha = -0.0141 \text{ kbar}^{-1}$ for InSb. Thus, the computer calculations appear to be consistent with analytical expressions. Therefore, for HgSe the same computer technique as used in analyzing the InSb data will be employed.

Values of $E_g = -0.22 \text{ eV}$, $P = 7.2 \times 10^{-8} \text{ eV cm}$, and higher band parameters of $B_1 = 0$, $B_3 = -3.5$, $L' = -2$, $M' = -5$, $N' = -1$, in units of $\hbar^2/2m_0$, $C_2 = -1.0 \text{ eV}$, and $(\hat{a} + C_1) = -6.5 \text{ eV}$, will be used in all the remaining HgSe calculations. The reasons for choosing these particular values of $B_3$ and $C_2$ will be discussed in a later section.

Thus, the solid lines in Fig. 23 represent the best-fit theoretical curves that result from using the deformation potentials $b = -1.6 \text{ eV}$ and $d = -2.7 \text{ eV}$, and a value of $\alpha = -0.193 \text{ kilobar}^{-1}$. Note that in the stress region investigated there is good agreement between data and theory.
Although the changes in the data appear to be almost linear and a definite curvature exists in the theoretical lines, the results lie within the experimental error. As will be seen later, the curvature of the theoretical lines diminishes as the concentration of the samples increase.

Next, consider sample #7 which has a concentration almost an order of magnitude larger than sample #1. Figures 24a, 24b, and 24c show reproductions of X-Y recorder tracings at various stresses for \(\sigma||[110]\). Comparing Fig. 21 and 24a, notice that the shift in peak position is much smaller for sample #7. The shifts in peak positions in #7 for \(B||[1\bar{1}1]\) and \(B||[110]\) are also smaller than those for sample #1. Figure 25 shows a plot of the fractional frequency changes versus stress for sample #7. Once again, the solid lines represent the best theoretical fit. The best-fit theoretical curves for sample #7 result from the deformation potentials \(b = -1.3e^{-V}\) and \(d = -2.7e^{-V}\), and a value of \(\alpha = -0.048\) kilobar\(^{-1}\). Note that for this sample, the curvature of the theoretical lines is much less than for sample #1. Also note how the absolute magnitude of the fractional frequency shifts has decreased with an increase in the crystal's concentration.
Fig. 24A--SdH Oscillations at Different Stress Values for Sample #7; $B \parallel [001]$. 
Fig. 24b—SdH Oscillations at Different Stress Values for Sample #7; $B \parallel [1\bar{1}1]$. 
Fig. 24c—SdH Oscillations at Different Stress Values for Sample #7; B∥[110].
Fig. 25--Fractional changes in SdH Frequency versus Stress for Sample #7; Solid Lines Represent Theoretical Predictions.
Next, let us pursue this line of thought to its logical end, that is, consider one of the highest concentration samples and look at its frequency changes. Although higher concentration samples were run, the highest concentration samples that gave good SdH data were approximately $3 \times 10^{18} \text{ cm}^{-3}$. In Fig. 26 the fractional frequency changes versus stress for sample #9 are plotted. The magnitude of the changes that occur in this concentration range are yet smaller than those observed for sample #7; thus the magnitude of the frequency shifts continues to decrease as the crystal's concentration increases. In sample #9 the fractional frequency change for $B || [110]$ has changed signs from that of sample #7. Now, as with the previously discussed samples, the solid lines in Fig. 26 represent the best-fit theoretical calculations for sample #9. This fit is obtained by using $b = -1.2eV$, $d = -2.7eV$, and $\alpha = -0.018 \text{ kilobar}^{-1}$.

In this section the magnitude of the frequency changes with stress have been shown to be a function of concentration, namely the lower the concentration the greater the frequency shifts when $\sigma || [110]$. Data has been specifically shown for three samples throughout the concentration range. Figure 27
Fig. 26--Fractional Changes in SdH Frequency versus Stress for Sample #9; Solid Lines Represent Theoretical Predictions.
Fig. 27--Fractional SdH Frequency Changes versus Concentration for $\sigma \parallel [110]$. 

SLOPE = $-\frac{2}{3}$
shows a plot of the concentration dependence of the magnitude of the frequency changes. Table III shows results of other data within the range of investigation. Two samples have been included in this table more for phenomenological than interpretative reasons. Notice samples \#2 and \#5 have different stress direction and therefore have fractional frequency changes that are different than those for a [110] stress direction. Data from \#2 indicate a larger change occurs for \textbf{B}||[\textbf{1\overline{1}}\textbf{0}] when \textbf{\sigma}||[\textbf{1\overline{1}}\textbf{1}] than when \textbf{\sigma}||[\textbf{110}]. On the other hand, sample \#5 displays a smaller change in frequency for \textbf{B}||[\textbf{001}] when \textbf{\sigma}||[\textbf{100}] than when \textbf{\sigma}||[\textbf{110}].

Thus, the experimental data exhibit a certain dependence upon stress direction.

While on the subject of the effects of stressing along different crystallographic directions, it would be informative to consider the variations between the energy bands as the stress direction is changed. Figures 28a, 28b, and 28c show plots of the change in energy between energy bands as a function of stress for different stress directions as calculated by the computer program in Appendix D. In these plots hh represents the heavy hold band while lc represents the light mass conduction band. These figures clearly show different variations of the energy bands for different stress directions.
### TABLE III

**SUMMARY OF SdH FREQUENCY (F) DATA**

<table>
<thead>
<tr>
<th>Sample Number</th>
<th>$F_{ave}^{\sigma=0}$ $(10^5 \text{ G})$</th>
<th>$n = (3.18 \times 10^6)^{3/2}$</th>
<th>$\Delta F/F$</th>
<th>Stress Direction</th>
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<tr>
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<td>$F_{ave} \times 10^{17} \text{ cm}^{-3}$</td>
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<td>B $</td>
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<td>-0.020</td>
<td>0.000</td>
</tr>
<tr>
<td>7</td>
<td>24.8</td>
<td>6.99</td>
<td>-0.023</td>
<td>0.010</td>
</tr>
<tr>
<td>8</td>
<td>23.8</td>
<td>6.59</td>
<td>-0.020</td>
<td>0.000</td>
</tr>
<tr>
<td>9</td>
<td>70.0</td>
<td>33.2</td>
<td>-0.007</td>
<td>0.004</td>
</tr>
<tr>
<td>10</td>
<td>68.5</td>
<td>32.1</td>
<td>-0.006</td>
<td>0.004</td>
</tr>
<tr>
<td>11</td>
<td>83.3</td>
<td>43.1</td>
<td>-0.006</td>
<td>0.004</td>
</tr>
</tbody>
</table>
Fig. 28a—Changes Between Energy Bands in HgSe for $\sigma \parallel [001]$. 
Fig. 28'b—Changes Between Energy Bands in HgSe for \( \sigma \parallel [\bar{1}10] \).
Fig. 28c - Changes Between Energy Bands in HgSe for $\sigma \parallel [1\overline{1}1]$. 
Orientation of Sample by Beats

As stated in section (5.1) the easiest and principle method used in this investigation for orienting a crystal in the plane of the magnetic field was that of beating effects. In this section the beating effect method of orientation is discussed. First, the crystal is prepared with a major crystallographic direction along its length (usually the [110] direction). With the [110] direction along the length of the sample, three major crystallographic directions ([001], [111], [110]) lie in a plane transverse to this [110] direction. While x-ray techniques can verify each individual direction, x-ray methods cannot be used once the sample is mounted in the stress apparatus. Since exact orientation cannot be maintained during mounting of the sample, another method for checking or determining orientation is desirable. While the absolute frequencies, as outlined in section (5.1), may be used, it is easier and more exact to use beating effects.

Figure 29 shows typical reproductions of x-y recorder tracings of SdH oscillations for different magnetic field directions. In this figure the beat position is first seen to increase as the field is rotated from 110° to a maximum
Fig. 29--Beats in SdH Oscillations for Different Magnetic Field Directions; [001]~128°.
field value at approximately 130°. Then, as the magnetic field direction continues to be rotated, the beat position drops to a lower magnetic field value. Depending upon concentration, beats may be seen in the vicinity of the [001] and [111] directions. If one plots the nodal position of a beat versus the magnetic field direction, the orientation of the sample may be determined. At zero stress only one nodal position has been seen when \( B \parallel [001] \), while two nodal positions have been seen \( B \parallel [1\bar{1}1] \). The nodal point with maximum field value occurs for a [1\bar{1}1] direction, while the node with the next largest field value occurs for a [001] direction. Another node occurs at still a lower field value when \( B \parallel [1\bar{1}1] \). This second or low-field [1\bar{1}1] beat does not possess a large angular anisotropy and is thus less useful for orientation purposes than the high field [111] beat\(^{13}\). Thus, orientation of the sample can be accomplished by plotting nodal position as a function of magnetic field direction. Figure 30 shows a plot of the nodal positions of three equivalent [111] beats versus the magnetic field direction for sample #4. From such a plot it is quite easy to determine the orientation of the [111], as well as the [001] and [110], directions.
Fig. 30--Beat Nodal Position versus Magnetic Field Direction.
Since the effect of stress is being considered in this investigation it would be advantageous at this point to discuss the effect stress has on the orientation plot of the HgSe beats. In Fig. 31 the nodal position of the beats versus magnetic field direction is shown for three different stress values. As can be seen from this plot, stress only shifts the relative position of the beats. The general shape of the curve remains approximately the same, particularly in the vicinity of the [111] beat. Thus both the stressed and unstressed beating effects in HgSe are a useful tool in determining sample orientation in a plane perpendicular to the stress direction. Although it will be discussed in detail in the next section, notice in Fig. 31 that the beat position in the [001] direction (178°) does not move in the same manner as the [111] beat (233°).

Beating Effects Under Stress

As previously mentioned, the problem of beating effects in HgSe is extremely complicated and complete understanding of all the experimental results at zero stress is lacking. In order to gain additional experimental data and thus aid in the understanding of the beating effects, uniaxial
Fig. 31--Beat Nodal Position versus Magnetic Field Direction; [111]~233°.
stress has been used to obtain new data that is relevant to this problem. Therefore, in this section uniaxial stress data on the beating effects will be presented and discussed.

First, at zero stress three nodal points are seen in the SdH oscillations of HgSe; one node occurs for $B \parallel [001]$ and two nodes are present when $B \parallel [1\bar{1}1]$. Under application of uniaxial stress the magnetic field positions of these nodal points are found to change. This fact has already been demonstrated to some degree in Fig. 31 in section (5.1). However, let us now consider these beat position changes in more detail. Reproductions of X-Y recorder tracings of the SdH oscillations in sample #8 when $B \parallel [1\bar{1}1]$ are shown in Fig. 32 for different stress values. In this figure the magnetic field value of the nodal point is seen to move to higher field values with the application of uniaxial stress. As mentioned earlier two beats occur when $B \parallel [1\bar{1}1]$, but notice only one nodal point is present in this figure. This is because the low field nodal position for this particular concentration is at a field value too low to observe good SdH oscillations. As the concentration of the samples increase the zero stress nodal positions of the beats increase in magnetic field value, and therefore this low
Fig. 32--SdH Oscillations of Sample #8 Showing Beat Movement with Stress; $B \parallel [111]$, (R. G. Stands for Relative Gain).
field nodal position becomes evident. Note the terminology low field beat and high field beat to distinguish the two nodes when \( B \parallel [\text{111}] \).

Next, in Fig. 33 reproductions of X-Y recorder tracings are shown for sample #8 when \( B \parallel [001] \) for 0 and 1 kilobar of stress. In this figure the beat position also moves to a higher magnetic field value with stress, but the amount of movement of the [001] nodal point is much less than the [1\overline{1}1] high field nodal point. The movement of a beat position with stress appears to be a general property of HgSe. Figure 34 shows a plot of the high field, [1\overline{1}1], beat nodal position versus [110] stress for several HgSe samples. From this plot, the high field [111] node is seen to experience the same shift regardless of the sample's concentration. At least this fact holds true throughout the majority of the concentration range investigated. For the higher concentration samples, the high field beat occurred at a magnetic field value beyond the capabilities of the instruments used; thus, exact verification of the beat movement at higher concentrations is lacking. However, extrapolation of the data presented in Fig. 34 would indicate a uniform movement of the high field [111] beat for all concentration
Fig. 33—SdH Oscillations Showing Beat Movement with Stress for Sample #8; $B \parallel [001]$, (R. G. Stands for Relative Gain).
Fig. 34—High-Field [111] Beat Nodal Position versus Stress for Different Samples.
ranges when the crystal is stressed along a [110] crystallo-
graphic direction.

Figure 35 shows a plot of the [001] nodal position as a function of stress for different samples. The circular data points are for a [110] stress direction and the square points are for a [100] stress direction. The [110] stress data presented in this figure suggest that the [001] beat has characteristics similar to the [111] high-field beat, that is, a uniform movement of the beat position with stress but relatively independent of concentration. While the change in nodal position appears to be uniform within the concentration range studies, the magnitude of the change in nodal position with stress (slopes of lines in Figs. 34 and 35) is greater for the [111] high-field beat. (The gap in the data for the [001] beat is due to the fact that no samples were obtainable within that particular concentration range.) Data from several samples are plotted as a function of concentration in Figs. 36 and 37. These data represent the high-field [111] beat and the [001] beat respectively.

Next, consider the square data points in Fig. 35 which represent data for stress along a [001] crystallographic direction. Once again this particular sample is included for
Fig. 35--[001] Beat Nodal Position versus Stress for Different Samples; Squares Represent \( \sigma \parallel [100] \), Triangles Represent "new" [001] Beat.
Fig. 36—Concentration Dependence of the High-Field [111] Nodal Positions.
Fig. 37—Concentration Dependence of the [001] Nodal Positions.
phenomenological rather than interpretative reasons. The raw data for sample #5 is shown in a reproduction of X-Y recorder tracings in Fig. 38. According to the data from sample #5, linear changes in the [001] beat position do not occur when the sample is stressed along a [100] direction. Thus, as with the frequency changes, the magnitude of the change in beat position with stress may vary depending upon the direction of uniaxial compression.

Up to this point the discussion has been limited to the [001] beat and the high-field [1L1] beat. Next, let us consider the low-field [1L1] beat. Recall that two beats occur when B∥[1L1]. Depending upon the sample's concentration and the instrumentation one or both of these beats may be observable. With the samples available for this investigation the low-field [1L1] beat was only observable in the higher concentration samples. Data from three samples are shown in Fig. 39 which illustrate the low-field [1L1] beat movement with stress. The data from sample #11 may be questionable, particularly since the sample broke at slightly above one-half kilobar of stress, and the samples are generally expected to withstand one kilobar of uniaxial stress. Sample #9 only has data points to three-quarters kilobar, but this
Fig. 38- [001] Beat Movement at Different Stress Values for $\sigma || [100]$.
Fig. 39--Low-Field [111] Beat Nodal Position versus Stress for Different Samples.
sample did not break until almost one kilobar of compression. Thus, there is little reason to question the data from sample #9.

Therefore, assuming samples #9 and #10 are representative of the low-field [111] beat, comparison can be made to the [001] and [111] high-field beat. The low-field [111] beat moves very little with stress while the high-field beat is subject to quite large changes in field values. Since some of the previous data can be explained by a semiclassical model and some by a quantum-mechanical model, a point of interest is the effect uniaxial stress has on the two [111] beats. If the two nodes seen for B‖[111] are connected by simple beating, more nodes should appear within the field range when the magnetic field is rotated from a [111] to a [110] direction. As seen in Fig. 30, no additional nodes are detectable. Thus, zero stress data implies that these two nodes are not connected by simple beating. Now, uniaxial stress allows further verification of this fact. If the nodal positions of the two [111] beats are related by simple beating, then the fractional changes of the nodal points would be expected to shift the same amount under stress. However, as seen in Figs. 34 and 39, this is not
the case. The high-field $[1\bar{1}1]$ beat changes much more under stress than the low-field beat. Thus in spite of the fact that the concentration dependence of the beat frequency for $B \parallel [1\bar{1}1]$ can be explained over the complete concentration range using a semiclassical theory, uniaxial stress data presents further proof that the two $[1\bar{1}1]$ nodes are not connected by simple beating and may be cited as evidence for an inadequacy of the semiclassical theory.

Only one beat or node has been previously seen for $B \parallel [001]$. In this investigation a second beat appeared in one of the higher concentration samples, #10, at approximately one-half kilobar when $B \parallel [001]$. Sometimes inhomogeneity beats may occur in a sample. However, this type of beat is detectable by its lack of angular anisotropy. This second beat observed in sample #10 displayed an anisotropy typical of a true beat. One other possible explanation of an unexpected beat is the interaction of the AC magnetic modulation field with the SdH oscillations. However, this type of beat is usually confined to the lower range of the D. C. Magnetic field values and is easily checked by observing the beat as the modulation field is changed. Thus, the new beat does not appear to be an inhomogeneity or modulation
field beat. Therefore, assuming this new [001] beat to be a real phenomena, consider its movement under stress and compare the two [001] beats. As with the two [111] beats, the movement of these [001] nodes with stress can determine whether or not these beats are connected by simple beating. Reproductions of X-Y recorder tracings are shown in Fig. 40 for sample #10. In this figure the original [001] beat is seen to move to higher field values (above 20kG) and the new [001] beat is seen to appear. The change in nodal position of this new [001] beat is shown by the triangular data points in Fig. 35. Comparison of the two curves for sample #10 in Fig. 35 indicates that the two nodal positions are changing by different amounts under stress and, hence, are not related by simple beating. Thus, the behavior of this second [001] beat under stress gives additional evidence for the inadequacy of the semiclassical theory.

Qualitatively the beats in InSb and their movement under application of uniaxial stress can be explained as shown in Chapter IV. The data from the InSb sample was fitted to the theory and values of $B_3$ and $C_2$ were estimated. The values of $B_3$ and $C_2$ determined for InSb are consistent with other measurements. In the case of HgSe, reasonable
Fig. 40--Appearance of Second [001] Beat under Application of Stress to Sample #10.
fits of the theory to data were not obtained throughout the concentration range. All of the attempts to fit the theory to the data give values of $B_3$ and $C_2$ that are inconsistent with other investigations. Thus, while the theory appears to give reasonable and consistent results for the InSb beating effects, more work needs to be done on this theory in order to explain the phenomena observed in HgSe. It was for this reason that the values of $B_3 = -3.5$, in units of $\hbar^2/2m_0$, and $C_2 = -1.0eV$ were chosen from other investigations.
CHAPTER VI

SUMMARY AND CONCLUSIONS

One of the points of concern from the beginning of this investigation was the determination of certain band parameters and the deformation potentials in InSb and HgSe. The theory outlined in Chapter II allows determination of these parameters. Since InSb is a more well-known material than HgSe, the above theory was first applied to InSb. Although the deformation potentials for InSb have been previously determined in other investigations, no previous study had verified the existence of beating effects in InSb. Thus, no value of the inversion-asymmetry splitting parameter has ever been reported even though the theoretical existence of this splitting is well-known. In Chapter IV the deformation potentials have been determined, as well as, the verification of the existence of beating effects in InSb. In addition the first reported value of the inversion-asymmetry splitting parameter has been given. The values of the parameters obtained in Chapter IV are as follows: $b = -1.8^{\pm} 0.2eV$. 

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\[ d = -2.2 \pm 0.4 \text{ eV}, \quad C_2 = -1.7 \pm 0.3 \text{ eV}, \quad \text{and} \quad B_3 = -3.3 \pm 0.5 \hbar^2/2m_0. \]

The value of \( b \) is in good agreement with previously reported values, but the value of \( d \) is somewhat smaller than expected. The reason for the difference in the values of \( d \) is not yet understood. Since the value of \( B_3 \) had not previously been determined for InSb, only a comparison to values for other materials could be made. This was done in Chapter IV and the values of \( B_3 \) and \( C_2 \) were found to be consistent with other measurements. Thus, the theory appears to explain the data for InSb.

Next, let us consider this theory when applied to HgSe. The value of \( b \) was found to be slightly concentration-dependent. The deformation potentials are expected to decrease as concentration increases. From the lowest to the highest concentration samples, the value of \( b \) varied from \(-1.2 \pm 0.3 \text{ eV} \) to \(-1.6 \pm 0.2 \text{ eV} \). A study of the concentration dependence of \( b \) in InSb could possibly add additional information on this point. The value of \( d \) was found to be \(-2.7 \pm 0.4 \text{ eV} \) throughout the concentration range. Since values for the deformation potentials in HgSe have never been reported, a comparison to a similar material is presented. In gray tin, which has the same type band structure as HgSe,
values of \( b = -1.9 \, \text{eV} \) and \( d = -3.3 \, \text{eV} \) have been reported for a concentration of \( 6 \times 10^{15} \, \text{cm}^{-3} \). Thus, the values reported in this study for HgSe are comparable to those obtained from gray tin. While the theory presented in this work appears to allow the determination of the deformation potentials in both InSb and HgSe, it only permits the splitting parameter to be evaluated in InSb. As discussed in Chapter V a consistent and reasonable fit of the semiclassical theory to the HgSe beat data was not obtainable. Possibly the inclusion of a fourth band and construction of an \( 8 \times 8 \) Hamiltonian would be beneficial in this regard.

Although unable to extract the splitting parameter from the beating effects data, the study of the magnetic-field positions of the beats under stress was useful for other reasons. The usefulness of these beats for orientational purposes in both stressed and unstressed HgSe was demonstrated in Chapter V. The high-field \([\overline{1}11]\) beat was shown to be the most useful for orientation of the sample.

Another point of interest was that theoretical work indicated that the Fermi surface of these types of semiconductors should become anisotropic under application of uniaxial stress, but no direct experimental proof for this
anisotropy had ever been given. In this paper evidence has been presented that shows that the Fermi surface of InSb and HgSe becomes anisotropic under application of uniaxial stress. This anisotropy in InSb was shown in Appendix D to be directly related to the deformation potentials, b and d, thus permitting their direct extraction from the data.

In conclusion, the theory and techniques presented in this investigation allows one to determine the deformation potentials in InSb and HgSe. This study also demonstrated the usefulness of this approach in determining the inversion-asymmetry splitting parameter in InSb type materials, but indicates additional work is necessary before it can be applied to the inverted band structure materials like HgSe. In addition, methods outlined in this investigation allow the anisotropy of the Fermi surface of these types of semiconductors to be investigated.
APPENDIX A

DIMENSIONAL CORRECTIONS

Since the Hall coefficient and resistivity depend upon sample dimensions, a change in these properties will occur due to the dimensional variations of a crystal under stress. These dimensional corrections have to be considered when making Hall and resistivity measurements with stress. Dimensional corrections for the D.C. Hall constant and D.C. resistivity are as follows:

\[
\frac{\Delta R_H}{R_H} = \frac{\Delta t}{t}, \quad (A-1)
\]

\[
\frac{\Delta \rho}{\rho} = \frac{\Delta w}{w} + \frac{\Delta t}{t} - \frac{\Delta \lambda}{\lambda}, \quad (A-2)
\]

where \(\lambda, w, t\) are the length, width, and thickness of the sample. For a cubic crystal the quantities on the right side of equs. (A-1) and (A-2) vary depending upon the direction of uniaxial compression. The relations for the various stress directions are as follows: (i) for
stress applied along a [100] direction,

\[ \frac{\Delta l}{l} = -\sigma S_{11}, \]  

\[ \frac{\Delta w}{w} = \frac{\Delta t}{t} = -\sigma S_{12}, \]  

(ii) for stress applied along the [111] direction,

\[ \frac{\Delta l}{l} = \frac{\sigma}{3} (S_{11} + 2S_{12} + S_{44}), \]  

\[ \frac{\Delta w}{w} + \frac{\Delta t}{t} = -\frac{\sigma}{3} (S_{11} + 2S_{12} - \frac{1}{2}S_{44}), \]  

(iii) For stress applied along the [110] direction,

\[ \frac{\Delta l}{l} = \frac{\sigma}{2} (S_{11} + S_{12} - \frac{1}{2}S_{44}), \]  

\[ \frac{\Delta w}{w} = \frac{\sigma}{2} (S_{11} + S_{12} - \frac{1}{2}S_{44}), \]  

\[ \frac{\Delta t}{t} = -\sigma S_{12}, \]  

where \( \sigma \) is the stress value and \( S_{ij} \) are the stiffness constants. The compliance constants, \( C_{ij} \), which are related to the stiffness constants, \( S_{ij} \), for HgSe have been determined by Lehoczky, et al.\(^{12}\). At 2\(^\circ\)K the
compliance constants are (in $10^{11}$ dynes/cm$^2$) $C_{11} = 6.898$, $C_{12} = 5.104$, $C_{44} = 2.307$. Thus, the stiffness constants can be determined using the above $C_{ij}$ values and the following relations:

\[
S_{11} = \frac{C_{11} + C_{12}}{(C_{11} - C_{12}) (C_{11} + 2C_{12})},
\]

\[
S_{12} = \frac{-C_{12}}{(C_{11} - C_{12}) (C_{11} + 2C_{12})},
\]

\[
S_{44} = \frac{1}{C_{44}^2},
\]

Hence, the $S_{ij}$ values are (in $10^{-11}$ cm$^2$/dyne) $S_{11} = 0.3911$, $S_{12} = -0.1663$, $S_{44} = 0.4334$.

Now, the dimensional corrections may be calculated for the various stress directions. As an example, consider the [110] stress direction. For HgSe at 0.5 Kbar,

\[
\frac{\Delta R_H}{R_H} = \frac{\Delta t}{t} = -\sigma S_{12} = 0.08 \times 10^{-2}
\]

and

\[
\frac{\Delta \varrho}{\varrho} = \frac{\Delta \varphi}{\varphi} + \frac{\Delta t}{t} - \frac{\Delta \lambda}{\lambda} = \sigma [1/2S_{44} - S_{12}] \text{ or } \frac{\Delta \varrho}{\varrho} = 0.19 \times 10^{-2}.
\]
APPENDIX B

COORDINATE TRANSFORMATIONS

The transformation of the \( k \) coordinates from a crystallographic coordinate system (where the \( k_x, k_y, \) and \( k_z \) axes is along the crystallographic axes) to a coordinate system in which one of the coordinate axes are along the magnetic field will be presented in this appendix. Generally, three cases are of importance, when the magnetic field, \( B \), is lying in a (100), (110), or (111) plane. The transformation for \( B \) lying in a (100) plane only requires one coordinate rotation, but for \( B \) lying in a (111) plane three rotations are required. As an example, the transformation for \( B \) lying in the (110) plane will be presented here is some detail, while only the results will be quoted for the other cases.

The crystallographic coordinate system will be labeled \( k_x, k_y, k_z \). The first rotation will be clockwise about the \( k_z \) axis through an angle \( (\gamma=45^\circ) \). This procedure will give new coordinate system \( k'_x, k'_y, k'_z \). Next, a counter clockwise rotation about the \( k_y \) axis through an angle \( \theta \).
defines the coordinate system \( k'' \), \( k''' \), \( k''' \). Mathematically, letting \( R_{ci} \) equal a clockwise rotation about the \( i \) axis and \( R_{cc} \) equal a counterclockwise rotation about the \( i \) axis, it follows that

\[
K' = R_{cz} K
\]  
\( (B-1) \)

and

\[
K'' = R_{ccy} R_{cz} K,
\]  
\( (B-2) \)

or rewriting eq. (B-2),

\[
K = R_{cz}^{-1} R_{ccy}^{-1} K'.
\]  
\( (B-3) \)

However, it can be shown that \( R_{cz}^{-1} = R_{ccz} \) and \( R_{ccy}^{-1} = R_{cy} \). Then eq. (B-3) becomes

\[
K = R_{ccz} R_{cy} K'.
\]  
\( (B-4) \)

If we substitute for the rotation matrices,

\[
\hat{K} = \begin{bmatrix}
\cos \gamma & \sin \gamma & 0 \\
-sin \gamma & \cos \gamma & 0 \\
0 & 0 & 1
\end{bmatrix}
\begin{bmatrix}
k''_x \\
k''_y \\
k''_z
\end{bmatrix}
\]  
\( (B-5) \)

which gives

\[
k''_x = k''_x \cos \theta \cos \gamma + k''_y \sin \gamma + k''_z \sin \theta \cos \gamma,
\]

\[
k''_y = -k''_x \cos \theta \sin \gamma + k''_y \cos \gamma - k''_z \sin \theta \sin \gamma,
\]

\[
k''_z = -k''_x \sin \theta + k''_y \cos \theta.
\]  
\( (B-6) \)
But, to get into the (110) plane take \( \gamma = 45^\circ \), and for the extremal cross-sectional area to occur in the plane, take \( k_z'' = 0 \). In addition introduce the polar coordinates \( k_\rho \) and \( \phi \), where \( k_x'' = k \cos \theta \), \( k_y'' = k \sin \theta \), \( k_z'' = 0 \). Then the equations in (B-6) become

\[
\begin{align*}
k_x &= \frac{k}{\sqrt{2}} \left( \cos \theta \cos \phi + \sin \phi \right), \\
k_y &= \frac{k}{\sqrt{2}} \left( -\cos \theta \cos \phi + \sin \phi \right), \\
k_z &= k_\rho \left( -\sin \theta \cos \phi \right). 
\end{align*}
\] (B-7)

Thus, \( \theta \) will be measured from the (001) crystallographic axis, and \( \phi \) from the (110) plane.

Similarly, for \( B \) lying in a (110) plane, \( \hat{R} = R_{cz} \hat{R}' \).

The results from this transformation are as follows:

\[
\begin{align*}
k_x &= -k_\rho \sin \theta \cos \phi , \\
k_y &= k_\rho \cos \theta \cos \phi , \\
k_z &= k_\rho \sin \phi , 
\end{align*}
\] (B-8)

where \( \theta \) is measured from the (100) axis and \( \phi \) from the (100) plane.

Likewise, performing three rotations gives the relations for \( B \) lying in a (111) plane, \( \hat{R} = R_{ccz} R_{ccx} R_{cz} \hat{R}'' \). These rotations give the following:
\[ k_x = \frac{k_p}{\sqrt{2}} [\cos\phi (\sin\theta + \cos\theta \cos\alpha) + \sin\phi (\sin\alpha)], \]

\[ k_y = \frac{k_p}{\sqrt{2}} [\cos\phi (-\sin\theta + \cos\theta \cos\alpha) + \sin\phi (\sin\alpha)], \]

\[ k_z = k_p [-\cos\theta \sin\alpha \cos\phi + \cos\alpha \sin\phi], \quad (B-9) \]

where \( \alpha = 54.8^\circ \), \( \theta \) is measured from the \((\overline{110})_a\) axis and \( \theta \) from the \((\overline{111}) \) plane.
The computer program used in this study will be presented here. The program consists of a main section with two subroutines. This program can be used to determine the eigenvalues of the matrix given in Chapter III; thus $E$ versus $k$ relations as a function of stress can be obtained. In addition the cross-sectional areas of the Fermi surfaces perpendicular to the magnetic field may be calculated. Also, a hundred and twenty points on the perimeter of each extremal Fermi surface cross section are obtained. This allows one to map the cross section of these surfaces. Examples of this are given in the main body of the thesis. From these areas the program calculates the Shubnikov-de Haas frequencies, the average frequency, and the beat frequency.

The subroutine MATSB is a revised program which was obtained from Mobil Research and Development Library in Dallas. The program appears in its modified form in this appendix. For the original program see P.A. Businger (77).
C PROGRAM TO FIND FREQ. & BEAT FREQ OF SDH OSC. FROM DIR & PIKUS
C 6TH DATA CARD IS ALPHA (CHANGE IN FERMI ENERGY)
C 1ST DATA CARD IS DETERMINATE SIZE & STRESS DIR., 100,111,110
C 2ND CARD IS EG,B1,B2,B3.
C 3RD CARD IS S11,S12,S44 (**ELASTIC CONSTANTS**) 
C 4TH CARD IS ALP(L'),AMP(M'),ANP(N')
C 5TH CARD IS C1,C2,ALA,ALB,ALC (DEFORMATION POTENTIALS)
C 6TH CARD IS THETA(B FIELD DIR), PHI, & CONCENTRATION(=/CM)
C 7TH CARD IS DEL(Delta), EF (FERMI ENERGY), ETOL (ENERGY TOLERANCE)
C 8TH CARD IS STRESS VALUE (SIGMA)

IMPLICIT REAL*4(A-H,O-Z)
REAL*8 X
DIMENSION X(6),AKRO1(121),AKRO2(121),XS(6)
COMMON//AR(20,20),AI(20,20),B1(20,20),AI(20,20),CR(20,20),
1CI(20,20),XR(20),XI(20),YR(20),Y1(20),ZR(20),ZI(20)
READ (05,3900) ALPHA
3900 FORMAT (E14.5)
READ 4000,M,DIR
4000 FORMAT(I3,F8.1)
5 READ (05,101) EG,B1,B2,B3
READ (05,103) S11,S12,S44.
BARH=0.38096E-15
101 FORMAT (4E14.5)
READ (C5,103) ALP,AMP,ANP
6 READ (C5,102) C1,C2,ALA,ALB,ALD
102 FORMAT (5E14.5)
WRITE (06,121)
121 FORMAT(// 9X,2HEG,12X,2HB1,12X,2HB2,12X,2HB3,//)
WRITE (06,107) EG,B1,B2,B3
107 FORMAT( 4E14.5,//)
WRITE (06,122)
122 FORMAT(// 9X,2HL',12X,2HM',12X,2HN',//)
WRITE (06,140) ALP,AMP,ANP
MDIR=DIR
B3=B3*BARH
ALP=ALP*BARH
AMP=AMP*BARH
ANP=ANP*BARH
WRITE (06,123)
123 FORMAT(// 9X,2HC1,12X,2HC2,12X,1HA,13X,1HB,13X,1HD,//)
WRITE (06,110) C1,C2,ALA,ALB,ALD
110 FORMAT( 5E14.5,//)
WRITE(06,57)
57 FORMAT(// ,9X,'S11',11X,'S12',11X,'S44',//)
WRITE(06,58) S11,S12,S44
58 FORMAT( 3E14.5)
8 READ(05,103) THETA,PHI,CON
READ 5070, DEL,EF,ETOL
5070 FORMAT(3E18.6)
EFF = EF
ROOK = (3.0 * (3.1416**2) * CON)**0.333
RHOK = ROOK
RAD = 57.2957795
ANGT = THETA / RAD
ANGP = PHI / RAD

103 FORMAT (3E14.5)
2 READ (05, 145) SIGMA
RHCK = ROOK
PHI = 0.0

145 FORMAT (E14.5)
555 WRITE (06, 141)
141 FORMAT ('*1', 10X, 'CON', 10X, 'KRHO', 9X, 'THETA', 10X, 'PHI', 5X,
          'STRESS DIR', 9X, 'SIGMA')
WRITE (06, 140) CON, RHOK, THETA, PHI, MDIR, SIGMA
140 FORMAT(*', 4E14.5, 5X, '*(', 13, '*')', 4X, E14.5)
WRITE (06, 5050)

IF (SIGMA.EQ.999.9) GO TO 201
IF (DIR-110.0) 14, 15, 16
14 EXX = -S11*SIGMA
EXY = 0.0
EXZ = 0.0
EYX = 0.0
EYY = -S12*SIGMA
EYZ = 0.0
EZX = 0.0
EZY = 0.0
EZZ = -S12*SIGMA

C (100) STRESS DIRECTION
GO TO 200

15 EXX = -(S11+S12)*SIGMA/2.0
EXY = -S44*SIGMA/4.0
EXZ = 0.0
EYX = EXY
EYY = EXX
EYZ = 0.0
EZX = 0.0
EZY = 0.0
EZZ = -S12*SIGMA

C (110) STRESS DIRECTION
GO TO 200

16 EXX = -(S11+2.0*S12)*SIGMA/3.0
EXY = -S44*SIGMA/5.0
EXZ = EXY
EYX = EXY
EYY = EXX
EYZ = 0.0
EZX = 0.0
EZY = 0.0
EZZ = -S12*SIGMA
EYY = EXX
EYZ = EXY
EZX = EXY
EZY = EXY
EZZ = EXX

C (111) STRESS DIRECTION

200  AKRC=0.0
210  EFTOL=ETOL*EF
220  PHI=0.0
230  KKK=0
240  LL=1
250  EF=EFF*(1.0+ALPHA*SIGMA)
260  DO 900 I=1,121
270    DELTA=DEL
280    NN=0
290    MM=0
300    JJ=0
310    JJJ=0
320  IF (LL-1) 6000,6000,6005
330  6000  RHOK=0.0
340  GO TO 500
350  6005  RHOK=ROOK
360  500  KKK=KKK+1
370  IF (DIR-110.0) 11,12,13
380      11  ALKX=-RHOK*COS(ANGP)*SIN(ANGT)
390      11  ALKY=RHOK*COS(ANGT)*COS(ANGP)
400      11  ALKZ=RHOK*SIN(ANGP)
410  GO TO 202
420      12  ALKX=(COS(ANGT)*COS(ANGP)+SIN(ANGP)/SQRT(2.0)
430      12  ALKY=(SIN(ANGT)+COS(ANGT)*COS(4ANGP))/RHOK/SQRT(2.0)
440      12  ALKZ=(-SIN(ANGT)*COS(ANGP))*RHOK
450  GO TO 202
460      13  BETA=54.8/RAD
470      13  ALKX=(COS(ANGP)*(SIN(ANGT)+COS(ANGT)*COS(BETA)))*RHOK/SQRT(2.0)
480      13  ALKY=(SIN(ANGT)+COS(ANGT)*COS(BETA))*RHOK/SQRT(2.0)
490      13  ALKZ=(-COS(ANGT)*SIN(BETA)*COS(ANGP)+COS(BETA)*SIN(ANGP))*RHOK
500  202  CONTINUE
510  ALK= SQRT(ALKX**2+ALKY**2+ALKZ**2)
520  LAMBA= EEX+EYY+EZZ
530  LAMXR= R3*ALKY+ALKZ+C1*EEE
540  AKXR= B3*ALKY+ALKZ+C2*EYZ
550  AKXY= B3*ALKZ+ALKX+C2*EZX
560  AKYI= B2*ALKY
570  AKYZ= B3*ALKX+ALKY+C2*EEX
580  AKZI= B2*ALKZ
590  AFPP= G.5*(ALP+AMP)*(ALKX**2+ALKY**2+ALKZ**2)+AMP*ALKZ**2+ALM*EZZ
\[ \text{AFP} = \text{AFPP} + 0.5 \times (\text{ALL} + \text{ALM}) \times (\text{EXX} + \text{EYY}) \]
\[ \text{AGPP} = (2.0/3.0) \times (\text{AMP} \times (\text{ALKX}**2 + \text{ALKY}**2) + \text{ALP} \times \text{ALK}**2 + \text{ALM} \times (\text{EXX} + \text{EYY})) \]
\[ \text{AGP} = \text{AFP} / 3.0 + \text{APP} + (2.0/3.0) \times \text{ALL} \]
\[ \text{AHPR} = -\text{ANP} \times \text{ALK} \times \text{ALKZ} + \text{ALN} \times \text{EXZ} / \text{SORT}(3.0) \]
\[ \text{AHPI} = -(\text{ANP} \times \text{ALKX} \times \text{ALKZ} + \text{ANP} \times \text{ALKX} \times \text{ALKY} \times \text{EXY}) / \text{SORT}(3.0) \]
\[ \text{AKPR} = (\text{AKXR} - \text{AKY}) / \text{SORT}(2.0) \]
\[ \text{AKPI} = (\text{AKXI} + \text{AKYR}) / \text{SORT}(2.0) \]
\[ \text{AKMR} = (\text{AKX} + \text{AKYR}) / \text{SORT}(2.0) \]
\[ \text{AKMP} = (\text{AKXI} - \text{AKYR}) / \text{SORT}(2.0) \]
\[ \text{CR}(1,1) = \text{LAMBA} \]
\[ \text{CR}(1,2) = 0.0 \]
\[ \text{CR}(1,3) = 0.0 \]
\[ \text{CR}(1,4) = -\text{AKPI} / \text{SORT}(3.0) \]
\[ \text{CR}(1,5) = (\text{SORT}(2.0/3.0)) \times \text{AKZ} \]
\[ \text{CR}(1,6) = -\text{AKM} \]
\[ \text{CR}(2,1) = 0.0 \]
\[ \text{CR}(2,2) = \text{LAMBA} \]
\[ \text{CR}(2,3) = \text{AKPR} \]
\[ \text{CR}(2,4) = \text{AKZI} \times \text{SORT}(2.0/3.0) \]
\[ \text{CR}(2,5) = \text{AKMR} / \text{SORT}(3.0) \]
\[ \text{CR}(2,6) = 0.0 \]
\[ \text{CR}(3,1) = 0.0 \]
\[ \text{CR}(3,2) = \text{AKPR} \]
\[ \text{CR}(3,3) = \text{AFP} \]
\[ \text{CR}(3,4) = \text{AHPR} \]
\[ \text{CR}(3,5) = \text{AIPR} \]
\[ \text{CR}(3,6) = 0.0 \]
\[ \text{CR}(4,1) = -\text{AKPI} / \text{SORT}(3.0) \]
\[ \text{CR}(4,2) = \text{AKZI} \times \text{SORT}(2.0/3.0) \]
\[ \text{CR}(4,3) = \text{AHPR} \]
\[ \text{CR}(4,4) = \text{AGP} \]
\[ \text{CR}(4,5) = 0.0 \]
\[ \text{CR}(4,6) = \text{AIPR} \]
\[ \text{CR}(5,1) = \text{AKZI} \times \text{SORT}(2.0/3.0) \]
\[ \text{CR}(5,2) = \text{AKMR} / \text{SORT}(3.0) \]
\[ \text{CR}(5,3) = \text{AIPR} \]
\[ \text{CR}(5,4) = 0.0 \]
\[ \text{CR}(5,5) = \text{AGP} \]
\[ \text{CR}(5,6) = -\text{AHPR} \]
\[ \text{CR}(6,1) = -\text{AKM} \]
\[ \text{CR}(6,2) = 0.0 \]
\[ \text{CR}(6,3) = 0.0 \]
\[ \text{CR}(6,4) = \text{AIPR} \]
\[ \text{CR}(6,5) = -\text{AHPR} \]
\[ \text{CR}(6,6) = \text{AFP} \]
\[ \text{CI}(1,1) = 0.0 \]
CI(1, 2) = 0.0
CI(1, 3) = 0.0
CI(1, 4) = AKPR/SQRT(3.0)
CI(1, 5) = AKZI*SORT(2.0/3.0)
CI(1, 6) = AKMR
CI(2, 1) = 0.0
CI(2, 2) = 0.0
CI(2, 3) = AKPI
CI(2, 4) = -AKZR*SQRT(2.0/3.0)
CI(2, 5) = AKMI/SQRT(3.0)
CI(2, 6) = 0.0
CI(3, 1) = 0.0
CI(3, 2) = -AKPI
CI(3, 3) = 0.0
CI(3, 4) = AIPI
CI(3, 5) = AIPI
CI(3, 6) = 0.0
CI(4, 1) = -AKPR/SQRT(3.0)
CI(4, 2) = AKZR*SQRT(2.0/3.0)
CI(4, 3) = -AIPI
CI(4, 4) = 0.0
CI(4, 5) = 0.0
CI(4, 6) = AIPI
CI(5, 1) = -AKZI*SORT(2.0/3.0)
CI(5, 2) = -AKMI/SQRT(3.0)
CI(5, 3) = -AIPI
CI(5, 4) = 0.0
CI(5, 5) = 0.0
CI(5, 6) = -AIPI
CI(6, 1) = -AKMR
CI(6, 2) = 0.0
CI(6, 3) = 0.0
CI(6, 4) = -AIPI
CI(6, 5) = AIPI
CI(6, 6) = 0.0
IEG = 0
IVEC = 0
IDET = 0
MIT = 100
MITS = 100
EP1 = 1.0E-4
EP2 = 1.0E-11
ALRS = 0.245
ALIS = 0.3E-08
GBR = 0.1
GBI = 0.1
CALL MATSB(IEG, IVEC, ALRS, ALIS, GBR, GBI, IDET, MIT, MITS, 1, EP1, EP2)
DO 666 II = 1, 6
666 X(II) = 1.0
N=6
K=1
ND=1
CALL SORT (X,N,K,ND)
C PRINT 5000
C5000 FORMAT ('O', 'ASCENDING EIGENVALUES')
DO 100 K=1,M
100 XS(K)=X(K)
C100 PRINT 5005,K,X(K)
C5005 FORMAT (6X,13,6X,E18.8)
IF (LL-1) 6001,6001,6008
6001 E5AO=XS(6)
   E5AO=XS(5)
   LL=2
   GO TO 6005
6008 CONTINUE
   IF (MM-250) 5021,5021,5099
5021 X5MEO=XS(5)-E5AO
   X6MEO=XS(6)-E6AO
   IF (JJJ.EQ.5) GO TO 604
   IF (ABS(EF-X6MEO)*LT.*ETOL) GO TO 601
   IF (EF-X6MEO) 600,601,602
602 RHOK=RHOK+DELTA*RHOK
   MM=MM+1
   JJ=3
   GO TO 500
600 RHOK=RHOK-DELTA*RHOK
   IF (JJ.EQ.3) GO TO 612
   IF (EF-X6MEO) 610,610,612
612 DELTA=DELTA/2.0
   RHOK=RHOK+DELTA*RHOK
610 MM=MM+1
   GO TO 500
601 AKRCI(I)=RHOK
   WRITE (06,5030) I,PHI,KKK,AKROI(I)
5030 FORMAT (' ',4,X,6,3X,F7.1,3X,16,3X,E16.7)
   JJ=0
   JJJ=5
   DELTA=DEL
604 IF (ABS(EF-X5MEO)*LT.*ETOL) GO TO 701
   IF (NN-250) 605,605,5099
605 IF (EF-X5MEO) 700,701,702
702 RHOK=RHOK+DELTA*RHOK
   NN=NN+1
   JJ=4
   GO TO 500
700 RHOK=RHOK-DELTA*RHOK
   IF (JJ.EQ.4) GO TO 712
   IF (EF-X5MEO) 710,710,712
712 DELTA=DELTA/2.0
RHOK = RHOK + DELTA * RHOK

710  NN = NN + 1
    GO TO 500

701  AKRC2(I) = RHOK
    WRITE(06, 5060) AKRO2(I)

5060  FORMAT(' ** ', A47X, E16.7)
    AKRC = AKRO1(I) + AKRC2(I) + AKRO
    PHI = PHI + 3.0

900  ANGP = PHI / RAD
    AKRC = AKRO / 242.0
    N = 120
    A = 0.0
    B = 360.0 / 57.2957795
    K = N + 1
    H = (B - A) / N
    ODD1 = 0.0
    ODD2 = 0.0
    EVEN2 = 0.0
    EVEN1 = 0.0
    DO 51 J = 2, N, 2
        EVEN1 = EVEN1 + (AKRO1(J))**2
        ODD1 = ODD1 + (AKRO1(J + 1))**2
        EVEN2 = EVEN2 + (AKRO2(J))**2
    51     ODD2 = ODD2 + (AKRO2(J + 1))**2
    AREA1 = ((AKRO1(1))**2 + 4.0 * EVEN1 + 2.0 * ODD1 - AKRO1(K)**2) +
            C * AKRO1(K)**2) * H / 6.0
    AREA2 = ((AKRO2(1))**2 + 4.0 * EVEN2 + 2.0 * ODD2 - AKRO2(K)**2) +
            C * AKRO2(K)**2) * H / 6.0
    FREQ1 = AREA1 / (9.544E+07)
    FREQ2 = AREA2 / (9.544E+07)
    CCNNN = (AKRO)**3 / (3.0 * 3.1416 * 3.1416)
    AVGFQ = (FREQ1 + FREQ2) / 2.0
    BEATF = (FREQ1 - FREQ2) / 2.0
    WRITE(06, 446)

446  FORMAT(' ** ', A3X, 'FERMI ENERGY', E6, 'EF', E6, 'EF TOLERANCE', E6, 'ETOL',
            C, '15X', 'DEL')
    WRITE(06, 447)

447  FORMAT(' ** ', A8, 'AREA1', A13, 'AREA2', A12, 'AVG RHO', A13, 'N')
    WRITE(06, 445) AREA1, AREA2, AKRO, CCNNN
    WRITE(06, 448)

448  FORMAT(' ** ', A8, 'FREQ1', A13, 'FREQ2', A13, 'AVG FREQ', A9, 'BEAT FREQ')
    WRITE(06, 445) FREQ1, FREQ2, AVGFQ, BEATF
    WRITE(06, 5091)

5091  FORMAT(' ** ', A9, 'STRESS DIRECTION', A2, '3 FIELD DIRECTION', A3, A9, 'STRESS VALUE', A12, 'ALPHA')
    WRITE(06, 5092) DIR, THETA, SIGMA, ALPHA

5092  FORMAT(' ** ', A9, 'FR.1', A11, A3E18.8)
GO TO 2
5099 WRITE (O6,5097)
5097 FORMAT (' ', 'NOT CONVERGED IN 250 VALUES OF RHOK')
201 STOP
END
OSUBROUTINE MABS \( (M, IEG, IVEC, ALRS, ALIS, GBR, GBI, IDET, MIT, CMITS, EP1, EP2) \)

ODIMENSION AR(20,20),AI(20,20),BR(20,20),BI(20,20),CR(20,20),
CI(20,20),XR(20),XI(20),YR(20),YI(20),ZR(20),ZI(20)

COMMON AR, AI, BR, BI, CR, CI, XR, XI, YR, YI, ZR, ZI

IONE=1
ITWO=2
N=M
SUMR=0.0
SUMI=0.0
PRDR=1.0
PRDI=0.0
TRACER=0.0
TRACEI=0.0
DO 450 I=1,N
TRACER=TRACER+CR(I,I)
450 TRACEI=TRACEI+CI(I,I)

C SET UP MATRICES
DO 519 I=1,N
XR(I)=0.
XI(I)=0.
YR(I)=0.
YI(I)=0.
ZR(I)=0.
ZI(I)=0.
DO 519 J=1,N
BR(I,J)=CR(I,J)
AR(I,J)=CR(I,J)
BI(I,J)=CI(I,J)
519 AI(I,J)=CI(I,J)

C EVALUATE DETERMINENT
ASSIGN 520 TO IA
ASSIGN 811 TO ID
MM=M
INTER=0
GO TO 535
520 DETR=1.0
DETI=0.0
DO 522 K=1,M
T1=DETR*AR(K,K)-DETI*AI(K,K)
DETI=DETR*AI(K,K)+DETI*AR(K,K)
522 DETR=T1
INTER=MOD(INTER,2)
IF (INTER) 1000,917,810
1000 STOP
810 DETR=-DETR
DETI=-DETI
917 GO TO 1D,(811,912)
C 811 PRINT 557,TRACER,TRACEI,DETR,DETI
C557 FORMAT(*0 TRACE OF MATRIX =*2E18.8,
DETERMINANT OF MATRIX = 2E18.8

CONTINUE

ASSIGN 912 TO ID
ASSIGN 530 TO IA
ASSIGN 40 TO IB
ASSIGN 523 TO IC
ISL = -1
GO TO 92

ISL = 0

EIGENVALUE GUESS OR ORIGIN TRANSLATION

ALR = ALRS
ALI = ALIS
IT = 1

EIGENVECTOR GUESS

DO 504 I = 1, N
XR(I) = 1.0
504 XI(I) = 0.0

DO 5 I = 1, N
AR(I, I) = AR(I, I) - ALR
5 AI(I, I) = AI(I, I) - ALI

FIRST ITERATION - POWER METHOD

IJ = 1

BIG = 0.

COMPUTE Y = (A - ALPHA) * X

DO 13 I = 1, N
YR(I) = 0.
YI(I) = 0.

DO 11 J = 1, N
YR(I) = YR(I) + AR(I, J) * XR(J) - AI(I, J) * XI(J)
11 YI(I) = YI(I) + AI(I, J) * XR(J) + AR(I, J) * XI(J)

AM = YR(I) ** 2 + YI(I) ** 2
IF (AM > BIG) GOTO 13, 13, 12
12 BIG = AM
JJ = I

CONTINUE

IF (BIG) GOTO 109, 106, 109

EXACT EIGENVALUE AND EIGENVECTOR - Y = 0. FLAG = 1000

ICT = 1000

DO 108 I = 1, N
JJ = I
IF (XR(I) > 1.0) GOTO 108, 118, 108

ISL = 1
GO TO 92

CONTINUE

PRINT 650
650 FORMAT (4BH ERROR. EIGENVECTOR NOT NORMALIZED IN METHOD 1.)
GO TO 990

MU RAYLEIGH QUOTIENT - (Y, X) / (X, X) = MU

RQNR = 0.
RON1 = 0.
RQD=0.
DO 14 I=1,N
RQNR=RQNR*XR(I)*YR(I)+XI(I)*YI(I)
RQNI=RQNI*XR(I)*YI(I)-XI(I)*YR(I)
14 RQD=RQD+XR(I)**2+XI(I)**2
AMUR=RQNR/RQD
AMUI=RQNI/RQD
AMM=AMUR**2+AMUI**2
IF (IEG) 1000,31,80
80 ALRC=AMUR+ALR
ALIC=AMUI+ALI
PRINT 300,IONE,IJ,ALRC,ALIC
300 FORMAT (2I4,2E20.8)
C TEST FIRST ITERATION
C MAGNITUDE OF (Y-MU*X)=TS
81 TS=0.
DO 15 I=1,N
150 TS=TS+(YR(I)-AMUR*XR(I)+AMUI*XI(I))**2+
1(YI(I)-AMUR*XI(I)-AMUI*XR(I))**2
C NORMALIZATION
DO 16 I=1,N
XR(I)=(YR(JJ)*YR(I)+YI(JJ)*YI(I))/BIG
16 XI(I)=(YR(JJ)*YI(I)-YI(JJ)*YR(I))/BIG
XR(JJ)=1.0
XI(JJ)=0.0
111 IF (TS/RQD-EP1) 2L,20,18
18 IF (IJ-MIT) 19,20,20
19 IJ=IJ+1
GO TO 10
C SECOND ITERATION - INVERSE POWER METHOD
20 ICT=IJ
MIT2=MITS+IJ
ALR=AMUR+ALR
ALI=AMUI+ALI
MM=N
DO 310 I=1,N
310 AI(I,I)=AR(I,I)-AMUR
GO TO 29
99 DO 100 I=1,N
29 IJ=IJ+1
C GAUSSIAN ELIMINATION - (A-ALPHA)*Y=X
IF(MM.LT.2) GO TO 2701
535 DO 27 I=2,MM
1 M1=I-1
DO 27 J=1,IM1
27 F=M=AR(I,J)**2+AI(I,J)**2
SM=SM**2+AI(J,J)**2
IF (FM-SM) 24, 24, 22
C
ROW INTERCHANGE - IF NECESSARY
22 DO 23 K=J, MM
T1 = AR(J, K)
T2 = AI(J, K)
AR(J, K) = AR(I, K)
AI(J, K) = AI(I, K)
AR(I, K) = T1
23 AI(I, K) = T2
T1 = XR(J)
T2 = XI(J)
XR(J) = XR(I)
XI(J) = XI(I)
XR(I) = T1
XI(I) = T2
T1 = FM
FM = SM
SM = T1
INTER = INTER + 1
24 IF (SM) 25, 27, 25
25 IF (FM) 90, 27, 90
C
TRIANGULARIZATION
90 RR = (AR(I, J) * AR(J, J) + AI(I, J) * AI(J, J)) / SM
RI = (AR(J, J) * AI(I, J) - AR(I, J) * AI(J, J)) / SM
DO 26 K = J, MM
AR(I, K) = AR(I, K) - RR * AR(J, K) + RI * AI(J, K)
26 AR(I, J) = 0.
AI(I, J) = 0.
XR(I) = XR(I) - RR * XR(J) + RI * XI(J)
XI(I) = XI(I) - RR * XI(J) - RI * XR(J)
27 CONTINUE
2701 GO TO IA, (520, 530, 911)
530 SMALL = 1000.
DO 28 K = 1, MM
IKK = K
T1 = AR(K, K) ** 2 + AI(K, K) ** 2
IF (T1) 750, 752, 750
750 IF (T1 - SMALL) 751, 28, 28
751 SMALL = T1
IZ = K
28 CONTINUE
GO TO IB, (46, 753)
752 IZ = IKK
IF (ISL) 753, 30, 30
C
EXACT EIGENVALUE - (A - ALPHA) SINGULAR. FLAG = 200C
30 ISL = 1
ICT = 2000
DO 974 I = 1, MM
XR(I) = 0.0
142

974 XI(I)=0.0
753 YR(IZ)=1.0
YI(IZ)=0.0
JJ=IZ
BIG=1.0
IF (IZ-MM) 33,32,33
32 IZZ=2
GO TO 95
33 IZZ=IZ+1
IF(IZZ.GT.MM) GO TO 3101
DO 31 I=IZZ,MM
YR(I)=0.
31 YI(I)=0.
3101 IZZ=MM-IZ+2
IF (IZ-1) 95,49,95
C BACKWARD SUBSTITUTION
40 IZZ=1
41 BIG=0.
IF(IZZ.GT.MM) GO TO 49
95 DO 46 I=IZZ,MM
II=MM-I+1
KK=II+1
SR=C.
SI=C.
IF (I-1) 42,44,42
42 IF(KK.GT.MM) GO TO 44
DO 43 K=KK,MM
SR=SR+AR(I,K)*YR(K)-AI(I,K)*YI(K)
43 SI=SI+AR(I,K)*YI(K)+AI(I,K)*YR(K)
44 T1=AR(I,I)*S1+AI(I,I)*S1
YR(I)=AR(I,I)*XR(I)-SR+AI(I,I)*(XI(I)-SI)/T1
YI(I)=AR(I,I)*XI(I)-SR-AI(I,I)*(XR(I)-SI)/T1
AM=YR(I)**2+YI(I)**2
IF (AM-BIG) 46,46,45
45 JJ=II
BIG=AM
46 CONTINUE
C NORMALIZATION - X=NORMALIZED Y
49 DO 47 I=1,MM
XR(I)=(YR(JJ)*YR(I)+YI(JJ)*YI(I))/BIG
47 XI(I)=(YR(JJ)*YI(I)-YI(JJ)*YR(I))/BIG
XR(JJ)=1.0
YI(JJ)=0.0
92 DO 601 I=1,N
DO 601 J=1,N
AR(I,J)=BR(I,J)
601 AI(I,J)=BI(I,J)
116 IF (ISL) 755,50,6C
755 GO TO 1C,(523,525,704)
C ALPHA RAYLEIGH QUOTIENT - (AX,X)/(X,X)=ALPHA
DO 52 I=1,N
   YR(I)=0.
   YI(I)=0.
   DO 51 K=1,N
      YR(I)=YR(I)+AR(I,K)*XR(K)-AI(I,K)*XI(K)
      YI(I)=YI(I)+AR(I,K)*XI(K)+AI(I,K)*XR(K)
      ALR=ALR+XR(I)*YR(I)+XI(I)*YI(I)
      ALI=ALI+XR(I)*YI(I)-XI(I)*YR(I)
   SUM=SUM+XR(I)**2+XI(I)**2
      ALR=ALR/SUM
      ALI=ALI/SUM
      AM=ALR**2+ALI**2
      IF (IEG) 1000,83,82
82  PRINT 300,ITWO,IJ,ALR,ALI
     C  TEST SECOND ITERATION
83  TS=0.
   DO 53 I=1,N
      T1=YR(I)-ALR*XR(I)+ALI*XI(I)
      T2=YI(I)-ALR*XI(I)-ALI*XR(I)
      TS=TS+T1**2+T2**2
   IF (TS/SUM-EP2) 60,60,301
301  IF (IJ-MIT2) 99,4G0,400
     PRINT 401,IT
     401 FORMAT (49H INVERSE POWER METHOD NOT CONVERGED ON TRY 1 )
      IF (IT-3) 402,990,402
     402  ALR=ALR+GBR
      ALI=ALI+GRI
      IT=IT+1
      PRINT 820,ALR,ALI
     820  FORMAT (11H ALPHA= 2E20.8)
      GO TO 4
60  ISL=0
   C 63  PRINT 64, N,ALR,ALI,ICT,IJ
   C 64  FORMAT (15H THE EIGENVALUE = 10X,E20.12,10X,E20.12,
               C15X,215 )
   63  CONTINUE
      ZR(N)=ALR
      ZII(N)=ALI
      SUMR=SUMR+ALR
      SUMI=SUMI+ALI
      T1=PRDR*ALR-PRDI*ALI
      PRDI=PRDR*ALI+PRDI*ALR
      PRDR=T1
   C  DEFLOATION OF MATRIX
      IF (JJ-N) 61,65,61
   C  PERMUTATION OPERATION
61  T1=XR(JJ)
\[
\begin{align*}
T2 & = XI(JJ) \\
XR(JJ) & = XR(N) \\
XI(JJ) & = XI(N) \\
XR(N) & = T1 \\
XI(N) & = T2 \\
\text{DO } 68 & \text{ K=1,N} \\
T1 & = AR(JJ,K) \\
T2 & = AI(JJ,K) \\
AR(JJ,K) & = AR(N,K) \\
AI(JJ,K) & = AI(N,K) \\
AR(N,K) & = T1 \\
68 & \text{ AI(N,K) = T2} \\
\text{DO } 62 & \text{ K=1,N} \\
T1 & = AR(K,JJ) \\
T2 & = AI(K,JJ) \\
AR(K,JJ) & = AR(K,N) \\
AI(K,JJ) & = AI(K,N) \\
AR(K,N) & = T1 \\
62 & \text{ AI(K,N) = T2} \\
\text{C DEFLATION} \\
65 & \text{ N=N-1} \\
\text{DO } 66 & \text{ I=1,N} \\
\text{DO } 66 & \text{ J=1,N} \\
AR(I,J) & = AR(I,J) - XR(I) \cdot AR(N+1,J) + XI(I) \cdot AI(N+1,J) \\
66 & \text{ AI(I,J) = AI(I,J) - XI(I) \cdot AR(N+1,J) + XR(I) \cdot AI(N+1,J)} \\
\text{DO } 600 & \text{ I=1,N} \\
\text{DO } 600 & \text{ J=1,N} \\
BR(I,J) & = AR(I,J) \\
600 & \text{ BI(I,J) = AI(I,J)} \\
\text{C COMPUTE EIGENVECTOR AND/OR DETERMINANT AS REQUIRED} \\
910 & \text{ IF } (IDET) 1000,527,700 \\
527 & \text{ IF } (IVEC) 1000,525,700 \\
700 & \text{ DO } 702 I=1,M \\
700 & \text{ DO } 702 J=1,M \\
AR(I,J) & = CR(I,J) \\
AI(I,J) & = CI(I,J) \\
\text{IF } (I-J) 702,701,702 \\
701 & \text{ AR(I,1) = AR(I,1) - ALR} \\
701 & \text{ AI(I,1) = AI(I,1) - ALI} \\
702 & \text{ CONTINUE} \\
MM & = M \\
INTER & = 0 \\
\text{ASSIGN 911 TO IA} \\
\text{GO TO 535} \\
911 & \text{ASSIGN 530 TO IA} \\
\text{IF } (IDET) 1000,914,520 \\
912 & \text{PRINT 913,DETR,DETI} \\
913 & \text{FORMAT (58X,12HDETERMINANT= 2E18.8)} \\
\text{ZLAG=SQRT (AR(1,1)**2+AI(1,1)**2)} \\
\text{ZLIT=ZLAG}
IF(M.LT.2) GO TO 9231
DO 923 I=2,M
ZMAGT=SQRT (AR(I,I)**2+AI(I,I)**2)
IF (ZLAG-ZMAGT) 922,920,920
920 IF (ZLIT-ZMAGT) 923,923,921
921 ZLIT=ZMAGT
GO TO 923
922 ZLAG=ZMAGT
923 CONTINUE
9231 PRINT924,ZLAG,ZLIT
924CFORMAT (45H LARGEST AND SMALLEST MAGNITUDES OF DIAGONAL C25HELEMENTS OF TRI. MATRIX = ,2E18.8/)
914 ISL=-1
IF (IVEC) 1000,916,915
915 DO 703 I=1,M
XR(I)=O.
703 XI(I)=O.
ASSIGN 753 TO IB
ASSIGN 704 TO IC
GO TO 530
916 ASSIGN 525 TO IC
GO TO 92
704 CONTINUE
PRINT705,(XR(I),XI(I),I=1,M)
705 FORMAT('0 ASSOCIATED EIGENVECTOR IS*/(2E25.14))
ASSIGN 40 TO IB
525 IF (N-1) 526,67,523
67 ALR=AR(1,1)
ALI=AI(1,1)
SUMR=SUMR+ALR
SUMI=SUMI+ALI
TI=PRDR*ALR-PRDI*ALI
PRDI=PRDR*ALI+PRDI*ALR
PRDR=TI
ZR(I)=ALR
ZII(I)=ALI
C PRINT 320,ALR,ALI
C320 FORMAT('1ST EIGENVALUE =',1UX,E20.12,1UX,E20.12,15X,C215/)
N=0
GO TO 910
526 CONTINUE
990 CONTINUE
RETURN
END
SUBROUTINE SORT (X, N, KK, ND)
IMPLICIT REAL * 8 (A-H,O-Z)
DIMENSION X(ND, 1)
K = IABS(KK)
J = N - 1
IF(J .EQ. 0) GO TO 55
IF(KK) 35, 55, 45
35 DO 20 M=1, J
   LC = M + 1
   DO 20 L=LC, N
      IF(X(K, M) - X(K, L)) 20, 20, 25
25 TEMP = X(K, M)
      X(K, M) = X(K, L)
      X(K, L) = TEMP
20 CONTINUE
RETURN
45 DO 50 M=1, J
   LU = M + 1
   DO 50 L=LU, N
      IF(X(M, K) - X(L, K)) 50, 50, 60
60 TEMP = X(M, K)
      X(M, K) = X(L, K)
      X(L, K) = TEMP
50 CONTINUE
55 RETURN
END
THE EFFECT OF STRAIN ON FERMI ENERGY

Since the Fermi energy changes with stress, it is necessary to include this shift in all of our calculations. In this section the method used to obtain this change in Fermi level will be outlined. The Hall data is found to vary only slightly with stress (~1% per kbar). Since most of this change can be accounted for by dimensional corrections, the change in the number of carriers with stress is negligible. Therefore, equating the analytical expressions for the number of carriers at zero stress, $N_0$, to the number of carriers with stress, $N_s$, will yield an expression for the stress dependent Fermi energy. In order to calculate $N_s$ it is necessary to write the energy in its ellipsoidal form and calculate the volume in k-space. The number of carriers can then be calculated from the volume.

First, using the energy relation Eq. (2.9) from Bir and Pikus$^{42}$ for stress along a [110] direction, we obtain
\[ E = \frac{\kappa^2}{2M^*} \left\{ k^2 \left( 1 - \frac{(a+C_1)\varepsilon}{E'_g} \right) + \frac{b}{2E'_g} \left( 3 \left( k_x^2 + k_y^2 \right) \varepsilon_{xx} + k_z^2 \varepsilon \right) \right\} + \frac{\sqrt{3} \sigma}{E'_g} (k_y k_x \varepsilon_{yx}) + C_1 \varepsilon + \frac{2 \varepsilon_{xy}}{E'_g}, \]  
where 
\[ \varepsilon = \begin{bmatrix} \varepsilon_{xx} & \varepsilon_{xy} & 0 \\ \varepsilon_{xy} & \varepsilon_{xx} & 0 \\ 0 & 0 & \varepsilon_{zz} \end{bmatrix}, \]  
\[ \frac{\kappa^2}{2M^*} = B_1 \frac{2B^2}{3E'_g}, \]  
\[ E'_g = E_g + E - C_1 \varepsilon = E_g + E'_f, \]  
and \( \varepsilon \) is the trace of \( \varepsilon \) matrix.

Next, isolating the coefficients in front of \( k_x^2, k_y^2, \) and \( k_z^2 \) will yield an ellipsoidal equation, \( K = A^* k_x^2 + B^* k_y^2 + C^* k_z^2 \), \( D^* k_x k_y \), where

\[ A^* = B^* \frac{1}{E'_g} - \frac{(a+C_1)\varepsilon}{E'_g} + \frac{3b \varepsilon_{xx}}{E'_g} - \frac{b \varepsilon}{2E'_g}, \]  
\[ C^* = 1 - \frac{(a+C_1)\varepsilon}{E'_g} + \frac{3b \varepsilon_{zz}}{E'_g} - \frac{b \varepsilon}{2E'_g}, \]  
\( D^* = k_x k_y \).
\[
D^* = \sqrt{3} \frac{\varepsilon_{yx}}{E'_g},
\]

\[
K = \left( E'_f - \frac{2C'_2}{3E'_g} \right) \frac{3E'_g}{2B'_2}.
\]

This ellipsoid may be transformed to the principal axis system which will yield

\[
1 = \frac{k^2_x}{a^2} + \frac{k^2_y}{b^2} + \frac{k^2_z}{c^2}
\]

where

\[
a^2 = \frac{K}{A^*+\frac{1}{2}D^*}, \quad b^2 = \frac{K}{A^*-\frac{1}{2}D^*}, \quad c^2 = \frac{K}{C^*}.
\]

Now, using eq. (D-5) and substituting appropriate values for the components of eq. (D-2), we have for small stresses

\[
\left(A^*+\frac{1}{2}D^*\right)^{1/2} = 1- \frac{(a+C_1) \varepsilon}{2E'_g} - \frac{(S_{11}-S_{12}) b \sigma}{8E'_g} - \frac{\sqrt{3} d S_{44} \sigma}{16 E'_g},
\]

\[
\left(A^*-\frac{1}{2}D^*\right)^{1/2} = 1- \frac{(a+C_1) \varepsilon}{2E'_g} - \frac{(S_{11}-S_{12}) b \sigma}{8E'_g} + \frac{\sqrt{3} d S_{44} \sigma}{16 E'_g},
\]

\[
c^{1/2} = 1- \frac{(a+C_1) \varepsilon}{2E_g} + \frac{(S_{11}-S_{12}) b \sigma}{4E'_g}.
\]

Next, one may calculate the volume of the ellipsoid using

\[
\text{Vol.} = \frac{4 \pi}{3} \ a^* b^* c^*.
\]

Substituting for \(a^*, b^*, c^*\) gives

\[
\text{Vol.} = \frac{4 \pi}{3} \ K^{3/2} \left( 1 - \frac{3/2 (a+C_1) \varepsilon}{E'_g} \right)
\]
where

\[ K = \frac{3E'_f E_g'}{3B_2^2} - \frac{C_2^2 \varepsilon_{yx}^2}{B_2^2}. \]

The total number of electron states, \( N_s = \frac{2}{8\pi^3} \text{Vol.} \)

Therefore,

\[ N_s(E^S_f) = \frac{\frac{1}{3\pi^2} \left( \frac{3}{2B_2^2} \right)^{3/2} (E_g + E^S_f)^{3/2} \left( \frac{2C_2^2 \varepsilon_{yx}^2}{3E_g'} \right)^{3/2}}{1 - \frac{3(a+C_1) \varepsilon}{2E_g'}} \]  

(D-9)

At zero stress all \( \varepsilon \) terms go to zero, Thus,

\[ N_o = \frac{1}{3\pi^2} \left( \frac{3}{2B_2^2} \right)^{3/2} \left[ E^O_f (E_g + E^O_f) \right]^{3/2} \]  

(D-10)

Now, equate \( N_o \) to \( N_s(E^S_f) \) and neglect terms of \( \varepsilon^2 \) and higher order, and solve for \( E^S_f \).

\[ E^S_f = -\frac{1}{2}(E_g + (a+C_1) \varepsilon) + \frac{1}{2} \left[ (E_g + (a+C_1) \varepsilon)^2 + 4E^O_f (E_g + E^O_f) \right]^{1/2} \]  

(D-11)

Where \( E_g' = E_g + E^S_f \) has been used.
From small stress this equation becomes

$$E_f^S = E_f^0 \left(1 - \frac{(a+C_1)\varepsilon}{E_g + 2E_f^0}\right)$$

(D-12)

Thus, the Fermi energy as a function of stress is calculated.

From equation (D-9) one may calculate the values of $a^*$, $b^*$, $c^*$. Then from these values the major cross-sectional areas can be calculated since

$$A_{001} = \pi a^*b^* \text{ for } B| [001],$$
$$A_{110} = \pi a^*c^* \text{ for } B| [110],$$
$$A_{111} = \pi b^*c^* \text{ for } B| [111].$$

(D-13)

From these areas, which are proportional to frequencies, one can obtain $\Delta F/F$ expressions.

First, consider $A_{001} = \pi a^*b^*$. The result of this calculation is

$$A_{001}(s) = A_o \left[1 + \frac{b(S_{11}-S_{12})g}{4(E_g+E_f^0)}\right]$$

(D-14)

where

$$A_o = \frac{3\pi}{2B_2} \left[E_f^0 E_g + E_f^0\right].$$

(D-15)
For the B11 [001] case
\[
\frac{\Delta F}{F} = \frac{b(S_{11} - S_{12})\sigma}{4(E_g + E_f^0)}.
\] (D-16)

Next using values appropriate for the sample investigated,
\[E_g = .235 \text{ e V} \quad \text{and} \quad E_f^0 = .0606 \text{ e V},\]
we find
\[
\frac{\Delta F}{F} = (2.56 \times 10^{-3})b.
\] (D-17)

Comparison to experimental data will then yield a value
for \(b\) of \(-1.7 \pm 0.1\).

In a similar manner, \(A_{110}\) may be computed. The results
are
\[
A_{110}(s) = A_0 \left( 1 - \frac{(a+C_1)\varepsilon}{E_{g=E_f^0}} \right) \left( \frac{(a+C_1)\varepsilon - b(S_{11} - S_{12})\sigma}{E_g'} + \frac{\sqrt{3}}{16E_g'} \frac{S_{44}\sigma}{d} \right).
\] (D-18)

The ratio \(F_{001}/F_{110}\) may now be constructed, and it gives
\[
\frac{F_{001}}{F_{110}} = 1 + \frac{3b(S_{11} - S_{12})\sigma}{8E_g'} - \frac{d \sqrt{3} S_{44}\sigma}{16E_g'}.
\] (D-19)

Again using appropriate values.
\[
\frac{F_{001}}{F_{110}} = 1 + [(3.84 \times 10^{-3})b - (1.17 \times 10^{-3})d] \sigma \quad (D-20)
\]

The term in brackets corresponds to the slope of the \( F_{001}/F_{110} \) line. From the experimental plot, the slope lies between \(-0.0036\) and \(-0.0045\). Thus, for a value of \( b = -1.7 \text{ eV} \), \( d \) becomes \(-2.1^{+0.4} \text{ eV} \), or for a value of \( b = -1.6 \), \( d = -1.8^{+0.4} \text{ eV} \).


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