The mobility, resistivity and carrier density in p-type silicon--etc.(u)

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THE MOBILITY, RESISTIVITY AND CARRIER DENSITY IN p-TYPE SILICON DOPED WITH BORON, GALLIUM AND INDIUM

By
Luis Carlos Linares

August 1979

Chairman: Sheng-San Li
Major Department: Electrical Engineering

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To verify our theoretical calculations, resistivity and Hall coefficient measurements were performed on silicon samples doped with boron, gallium and indium with dopant densities ranging from $4.25 \times 10^{15}$ to $9.07 \times 10^{17}$ cm$^{-3}$, for $100 \leq T \leq 400$ K, using planar square array test structures. Agreement between the calculated and measured resistivity values was within 10 percent over the range of temperatures and dopant density studied. Agreement between our calculated and experimental values of Hall mobility was within 15 percent for temperatures greater than 150 K. At 300 K, agreement between theoretical values of Hall factor and those deduced from experimental data of this work and that of other studies was within 15 percent for dopant densities greater.
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A DISSERTATION PRESENTED TO THE GRADUATE COUNCIL OF
THE UNIVERSITY OF FLORIDA
IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE
DEGREE OF DOCTOR OF PHILOSOPHY

UNIVERSITY OF FLORIDA
1979
TO MY FAMILY

FOR THEIR PATIENT SUPPORT
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\[ N_A = 6.44 \times 10^{16} \text{ cm}^{-3} \]

7.13 Hall factor vs dopant density for p-type silicon at 300 K
KEY TO SYMBOLS

A Inverse mass band parameter
A' Area of the base-collector diode
a Deformation potential constant (acoustic phonon scattering)
B Inverse mass band parameter
b Deformation potential constant (optical phonon scattering)
C Inverse mass band parameter
C_L Longitudinal sound velocity in silicon
C_T Transverse sound velocity in silicon
E Energy of holes
e Magnitude of the electronic charge
E_A Acceptor impurity energy level
E_F Fermi energy level
E_V Valence band edge
E_1 Binding energy of neutral acceptors
f_0 The Fermi-Dirac function
F_{1/2} Fermi-Dirac integral of order 1/2
g Ground state degeneracy
\hbar Plank's constant divided by 2\pi
I Current
J Current density
K Wave vector
k_0 Boltzmann's constant
$m_1$  Heavy-hole mass at 4.2 K

$m_2$  Light-hole mass at 4.2 K

$m_C^*$  Conductivity effective mass in the combined band

$m_{Ci}^*$  Conductivity effective mass in band $i$

$m_D^*$  Density-of-state effective mass in the combined band

$m_{Di}^*$  Density-of-state effective mass in band $i$

$m_G^*$  Geometric mean mass

$m_H^*$  Hall effective mass in the combined band

$m_{Hi}^*$  Hall effective mass in band $i$

$N_A$  Total acceptor impurity density

$N_{A^+}$  Ionized acceptor impurity density

$N_N$  Neutral impurity density

$n_o$  Phonon distribution function

$N_V$  Effective density of valence band states

$p_i$  Hole density in band $i$

$p'$  Effective screening hole density

$r_{Ai}$  Mass anisotropy factor in band $i$

$R_H$  Hall coefficient in the combined band

$r_H$  The Hall factor in the combined band

$R_{Hi}$  Hall coefficient in band $i$

$r_{Hi}$  The Hall factor in band $i$

$r_{Si}$  Scattering factor in band $i$

$S$  Probe spacing

$T$  Absolute temperature

$V$  Voltage

$V_H$  Hall voltage
Thickness of the chip
β Ratio of deformation potential constants
γ Function of band mass parameters
γ_{ij} Ratio of density-of-state effective masses
γ_{hh}^{a} Hole-hole reduction factor for acoustic phonon scattering
γ_{hh}^{i} Hole-hole reduction factor for ionized impurity scattering
γ_{hh}^{o} Hole-hole reduction factor for optical phonon scattering
Δ Energy of spin orbit splitting
ε Reduced energy \((E/k_{B}T)\)
ε_1 Variable of integration
ε_2 Variable of integration
ε_s Relative dielectric constant
ζ Limit of integration
η Reduced Fermi-energy
η_1 Scaling factor
θ Spherical coordinate
θ_D Debye temperature
\(\mu_{C}\) Conductivity mobility in the combined band
\(\mu_{Cl}\) Conductivity mobility in band \(i\)
\(\mu_{H}\) Hall mobility in the combined band
ξ Limit of integration defined in Figure 2.1
ρ Resistivity of holes
ρ_{S} Density of silicon
\(\sigma_{C}\) Electrical conductivity
\(\sigma_{H}\) Hall conductivity
\(\tau\) Total scattering relaxation time
\(\tau_{aci}\) Acoustic phonon scattering relaxation time in band \(i\)
\( \tau_{ii} \)  Ionized impurity scattering relaxation time in band \( i \)
\( \tau_{ij} \)  Total interband scattering relaxation time
\( \tau_{ii} \)  Total intraband scattering relaxation time
\( \tau_{Ni} \)  Neutral impurity scattering relaxation time in band \( i \)
\( \tau_{oi} \)  Optical phonon scattering relaxation time in band \( i \)
\( \tau_{x} \)  Adjustable scattering constant
\( \phi \)  Spherical coordinate
Using the relaxation time approximation and a three-band model (i.e., nonparabolic light-hole band, parabolic heavy-hole and split-off bands), a derivation involving the use of the Boltzmann transport theory was applied to obtain expressions for the valence band density-of-states effective mass, $m_D^*$, the valence band conductivity effective mass, $m_C^*$, and the valence band Hall effective mass, $m_H^*$, of holes in p-type silicon. Values of effective mass calculated from this model reveal the temperature and dopant density dependence of the effective mass due to the nonparabolic shape of the bands. With these values of effective mass and the three-band model, theoretical calculations of hole mobility, resistivity, Hall factor and Hall mobility were conducted for p-type silicon doped with boron, gallium and indium for dopant densities from $10^{14}$ to $10^{18}$ cm$^{-3}$ and temperatures between 100 and 400 K. Scattering contributions from acoustical and optical phonons, and ionized and neutral impurities were considered. In addition, interband scattering...
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factor and those deduced from experimental data of this work and that
of other studies was within 15 percent for dopant densities greater
than $5 \times 10^{16}$ cm$^{-3}$. From the results of this study, we conclude that the theoretical model and expressions developed here can accurately describe the mobility and resistivity in p-type silicon. The omission of band anisotropy considerations, however, introduces considerable error in the evaluation of the Hall factor for low dopant densities.
CHAPTER I
INTRODUCTION

The goal of this study has been to measure and compare with theory the resistivity and Hall mobility of holes in silicon doped with gallium and indium as functions of temperature and dopant density. Data taken on boron-doped silicon was also included in order to further confirm the adequacy of the theoretical model. In order to determine theoretically the resistivity and Hall mobility, one must first calculate the conductivity mobility, the density of holes, and the Hall factor. This can only be done with a thorough understanding of the energy band structure, the scattering mechanisms involved, and the carrier statistics.

The application of an electric or a magnetic field to a crystal results in a variety of carrier transport phenomena. These phenomena are associated with the motion of current carriers in the conduction or valence bands. The free charge carriers in a semiconductor will acquire a drift velocity under the influence of an applied electric field. This velocity is the net result of the momentum gained from the externally applied field, and the momentum lost in collisions which tend to randomize the carrier momentum [1]. If the field is expressed in volts per centimeter, and the velocity in centimeters per second, a mobility is defined as the incremental average speed per unit electric field, and is expressed in squared centimeters per volt second. The velocity, and consequently the mobility, is determined by the different types of collisions which the carriers undergo. Collisions of carriers with lattice atoms which
are out of their equilibrium positions because of thermal vibration, provide an upper limit to the mobility. Scattering of the carriers is also caused by impurities, both ionized and neutral. At high temperatures and low dopant densities, scattering by lattice phonons is more effective while at low temperatures and high impurity densities, scattering by ionized and neutral impurities predominates. In addition, the effects of hole-hole scattering on the lattice and ionized impurity scattering mechanisms need to be considered. Thus in calculating the mobility over a wide range of temperatures and dopant densities, all the different scattering mechanisms must be taken into account. Besides the mobility, the density of holes enters the problem of determining the electrical resistivity. The density of holes associated with dopant atoms is a function of the ionization energy of the dopant atom, the temperature, and the degeneracy factor. Calculation of the Hall mobility requires knowledge of the Hall factor which is a function of the scattering mechanisms and effective masses.

For purposes of device design it is necessary to know the correct relationship between the resistivity and dopant density at different temperatures. Evaluation of the characteristics of semiconductor devices and the study of transport phenomena in semiconductors requires an accurate knowledge of variations in the effective mass, mobility, and carrier density with changes in temperature and dopant density. Because of this, numerous studies of mobility, resistivity, and hole density in p-type silicon have been conducted [1-16]. However, due to the complexity of the valence band of silicon and the various scattering mechanisms involved, these studies, for the most part, have either been conducted in temperature and dopant density ranges designed to explore only a
particular type of scattering mechanism, or have not advanced the theory necessary to describe the experimental result. For example, Costato and Reggiani [4] calculated the mobility of holes for pure p-type silicon in which lattice scattering dominates; Braggins [1] considered nonparabolicity and all the relevant scattering mechanisms with the exception of hole-hole scattering, but he limited his investigation to dopant densities below $5 \times 10^{16}$ cm$^{-3}$ and low temperatures; Morin and Maita [5] considered wide ranges of temperature and dopant densities, but did not provide a theoretical examination of the data. Recently, Li [17] developed a theoretical model capable of describing the mobility and resistivity of p-type silicon over a wide range of temperatures and dopant densities. This improved model was applied to the case of boron-doped silicon with great success [17]. The improvement in the theory consisted mainly of the inclusion of hole-hole scattering effects, and consideration of the nonparabolic nature of the bands. In this study, Li's model [17] has been improved by including consideration of interband scattering effects on the acoustic phonon scattering mechanism, and has been applied to the study of silicon doped with impurities other than boron.

With some exceptions [14-16], most of the research in p-type silicon has been conducted with boron as the doping impurity, since boron is the shallowest acceptor in silicon and this material is widely available. A very limited amount of data is available on silicon doped with deeper impurities such as gallium and indium. These dopants, especially indium, are of great interest to modern technology because of their application to photo-detector devices. Curves of resistivity and mobility as functions of dopant density [2,3] have been applied to characterizing boron-doped starting material and diffused boron layers in silicon, and
have been found highly useful. Similar curves developed in this research may be expected to be equally useful for characterizing and integrating infrared detectors based on the deeper levels of indium and gallium with on-chip silicon electronics. Application of a more complete theory of mobility and resistivity [17] to the case of silicon doped with gallium and indium should provide an accurate description of the transport of holes in this material. These results may be of significant use in the study and design of infrared photo-detector devices.

In this research the mobility, resistivity, and hole density have been studied over a temperature range from 100 to 400 K and dopant densities from $4.25 \times 10^{15}$ to $9.05 \times 10^{17}$ cm$^{-3}$. Because of the complexity brought about by heavy doping effects and uncertainties in accounting for hole density and impurity density at high dopant densities, the theoretical analysis has been restricted to densities below $10^{18}$ cm$^{-3}$ in which the use of Boltzmann statistics is justified. The nonparabolic nature of the valence band structure, and derivation of expressions for the temperature dependent effective masses are presented in Chapter II. Since effective mass is directly related to the shape of the valence bands, the result is an effective mass which varies with temperature and dopant density. The mobility formulation includes consideration of the relevant scattering mechanisms and how these are modified by hole-hole scattering effects. These scattering mechanisms are considered in detail in Chapter III. Since the different scattering mechanisms which contribute to the mobility have different temperature and energy dependences, the use of numerical methods and curve fitting has been applied in analyzing the data. The temperature and dopant density dependence of resistivity and hole density is analyzed in Chapter IV. In Chapter V,
the Hall factor is discussed, and theoretical calculations of Hall mobility are presented. Fabrication techniques and experimental procedures are described in Chapter VI. Comparisons of experimental results with predictions based on the theory of Chapters III through V are made in Chapter VII; in this chapter the theoretical results are also compared with data published by other workers. Chapter VIII summarizes the research and states the main conclusions derived from this work.
CHAPTER II
BAND STRUCTURE AND EFFECTIVE MASS

2.1 Introduction

The interpretation of transport properties in silicon and the modeling of silicon junction devices depend on an accurate knowledge of values of effective mass. The complex valence band structure of silicon leads to difficulties in the study of transport properties of holes in this material. Thus the development of a model incorporating the nonparabolic nature of the band into a single parameter, the combined hole effective mass, would greatly simplify the study of mobility, resistivity, and the Hall effect in silicon. Including the band nonparabolicity in calculations of relaxation time via the effective mass formulation is a reasonable procedure and has been applied effectively by Radcliffe [18] to study acoustic phonon scattering, and by Barrie [19] to study optical phonon and impurity scattering in nonparabolic bands. In this chapter we will derive such a theoretical model for hole effective mass calculations in silicon.

Lax and Mavroides [20] have derived expressions for density-of-states effective masses $m^*_{D_1}$ and $m^*_{D_2}$ for the heavy-hole band and the light-hole band, respectively, which lead to the generally accepted and quoted value, $m^*_D = 0.591 m_o$. This value, however, can only be considered applicable at 4.2 K, where $m^*_1 = 0.537 m_o$ and $m^*_2 = 0.153 m_o$. A number of experimental data has been published which indicates both electron and hole effective mass to be dependent both on temperature and dopant
Below 50 K, hole effective mass remains constant as indicated in high frequency magnetoconductivity experiments [23]. However, at higher temperatures and for higher acceptor impurity densities, two mechanisms are responsible for the temperature dependence of the effective mass: the thermal expansion of the lattice, and the explicit effect of temperature. The effect of the thermal expansion can be estimated from the stress dependence of the effective mass [24], and has been shown to be negligible [21,25]. The explicit temperature effect however, is of great importance. It consists of three parts: (a) the temperature variation of the Fermi distribution function in a nonparabolic band, (b) the temperature dependent distribution function of the split-off band, and (c) the temperature variation of the curvature at the band extremum due to the interaction between holes and lattice phonons.

Following the work of Lax and Mavroides [20], but using Fermi-Dirac statistics and a simplified model of the valence band structure for silicon, Barber [25] obtained an expression for the density-of-states effective mass, $m^*$, which is temperature and hole-density dependent. Barber, however, did not apply the nonparabolic model of the valence band to the study of conductivity or Hall effective mass in p-type silicon. Costato and Reggiani [26] also developed expressions for $m^*$ and $m^*$, the band conductivity effective mass, which show a variation with temperature, but they neglected the effects of the split-off band and the temperature variation of the band curvature.

In this study, the expressions for density-of-states effective mass, conductivity effective mass, and Hall effective mass of holes are derived based on the following definitions. The density-of-states effective
mass, $m^*$, enters in the normalization of the distribution function; the conductivity effective mass, $m^*_c$, is the mass of a mobile charge carrier under the influence of an external electric field; and the Hall effective mass, $m^*_H$, is the mass of a mobile charge carrier under the application of external electric and magnetic fields. The reason for these particular definitions of effective masses is that the primary application of this work is to generate improved theoretical calculations of Hall mobility, resistivity, and conductivity mobility [17]. The derived expressions were used to calculate hole effective masses in p-type silicon over a wide range of temperature and dopant density. Since the crystal structure of silicon has cubic symmetry, the ohmic mobility and the low-field Hall coefficient are isotropic. An angular average of the effective masses may be performed taking into account separately the warping of the individual bands so that expressions for $m^*_D$, $m^*_C$, and $m^*_H$ of isotropic form can be derived. Values calculated from these expressions differ from one another because of the warping and nonparabolicity, and consequently effective mass in each band depends on temperature and dopant density in its own way. The valence band structure of silicon is presented in Section 2.2, and in Section 2.3 expressions for $m^*_D$, $m^*_C$, and $m^*_H$ are derived.

2.2 The Valence Band Structure of Silicon

Theoretical calculations by Kane [27] have established some basic features of the valence band of silicon. It consists of heavy-hole and light-hole bands, degenerate at $\overline{k} = 0$, and a third band displaced down in energy at $\overline{k} = 0$ by spin orbit coupling.

The heavy-hole band is characterized by holes with an energy independent, but direction-dependent effective mass. The light-hole band
is characterized by holes with an energy and direction-dependent effective mass. These two bands can be described by the \( E \) vs \( k \) relationship [28]

\[
E(k) = \frac{-\hbar^2}{2m_0} \left\{ A k_x^2 + \left[ B^2 k_y^4 + c^2 (k_x^2 k_y^2 + k_y^2 k_x^2 + k_x^2 k_z^2) \right] \right\}^{\frac{1}{2}}
\]

(2.1)

where \( A, B, \) and \( C \) are the experimentally determined inverse mass band parameters, \( k = (k_x^2 + k_y^2 + k_z^2)^{\frac{1}{2}} \), and the upper sign is associated with the holes in the light-hole band, while the lower sign is associated with the holes in the heavy-hole band. Values of \( A, B, \) and \( C \) are obtained by cyclotron resonance measurements at 4 K [22,29].

Although warped, the bands are parabolic for small values of \( k \). However, for larger values of \( k \), the bands become nonparabolic, and along the \( <100> \) and \( <111> \) directions the heavy- and light-hole bands are parallel over most of the Brillouin zone. This situation, however, is not strictly valid for general directions [30]. The assumption of overall parallelism, while questionable in III-V compounds, is reasonable in the case of Ge and Si [27,31]. The split-off band is separated at \( k = 0 \) by an energy \( \Delta = 0.044 \) eV. [32], and is characterized by an effective mass which is independent of energy and direction. If the anisotropy is small, the square root in equation (2.1) may be expanded [20] and the energy surfaces may be expressed by

\[
E = E_v - \frac{\hbar^2 k^2}{2m_0} (A \pm B') j(\varphi, \psi)
\]

(2.2)

where
\[ B' = (B^2 + C^2/6)^{1/2} \] \hspace{1cm} (2.3)

\( \theta \) and \( \phi \) are the spherical coordinates, \( E_V \) is the top of the valence band, and

\[ j(\theta, \phi) = 1 + \frac{1}{2} \gamma [\sin^4 \theta (\cos^4 \phi + \sin^4 \phi) + \cos^4 \theta - 2/3] \] \hspace{1cm} (2.4)

with

\[ \gamma = \frac{1}{2} C^2/2B'(A \pm B') \] \hspace{1cm} (2.5)

Following the work of Barber [25], we have used the simplified model of the band structure illustrated in Figure 2.1. In this model the heavy-hole band is considered parabolic and thus the mass \( m_1^* \) is a constant, equal to its value at 4.2 K. For energies within 0.02 eV the light-hole band is considered parabolic with a constant slope corresponding to the value of \( m_2^* \) at 4.2 K. For higher energies the light-hole band is assumed to take on approximately the same slope as that of the heavy-hole band, but remains separated from the heavy-hole band by \( \Delta/3 \) eV [27]. The extrapolation of these two constant slopes creates the kink in the light-hole band at 0.02 eV. Because of the change in slope, the light-hole band has an energy-varying effective mass and in general can only be described in terms of partial Fermi-Dirac integrals [25]. Although the split-off band is parabolically distributed, the apparent effective mass at the top of the valence band is a function of temperature due to the energy displacement at \( \overline{k} = 0 \). Theoretical and experimental studies [33,34] have shown that at high temperatures the heavy-hole band is not parabolic and thus \( m_1^* \) is not energy and temperature independent. However, within the range of
Figure 2.1. Simplified valence band structure of silicon based on Kane's [27] calculations and measured properties of the valence band.
temperatures considered here, the assumption of parabolicity for the heavy-hole band based on Kane's model [27] is reasonable. Other studies [35, 36] support the validity of this model for the valence band of silicon.

2.3 Effective Mass Formulation

In the case of spherically symmetric energy surfaces all of the carriers respond in the same way to a given set of applied forces. The effective mass then acts as a scalar and thus has the same value for the Hall effect, conductivity, and density of states. For nonspherical energy surfaces, however, this is not the case. The mixed response of carriers to a set of applied forces is reflected in differences between the different kinds of effective masses. The density-of-states effective mass, \( m_{\text{D1}}^* \), is defined from the relationship

\[
P_i = \frac{4}{\sqrt{\pi}} \left[ \frac{2\pi k_o T m_{\text{D1}}^*}{h^2} \right]^{3/2} F_{1/2}(\eta) \tag{2.6}
\]

where

\[
F_{1/2}(\eta) = \int_{-\infty}^{0} \frac{\varepsilon^i d\varepsilon}{T + \exp(\varepsilon - \eta)} \tag{2.7}
\]

\( \varepsilon = (E_V - E)/k_o T, \eta = (E_V - E_F)/k_o T, k_o \) is the Boltzmann constant, \( E_V \) is the top of the valence band, and \( i = 1, 2, 3 \) refers to the heavy-hole, light-hole, and split-off bands, respectively.

The electric current density in the presence of electric and magnetic fields can be expressed by [20]

\[
J_j = \sigma_{jk} E_k + \sigma_{jk} E_k H_L + \sigma_{jk} m_k H_k H_m + \ldots \tag{2.8}
\]
where $E_k$, $H_k$, $H_m$ are the electrical and magnetic field components and the $a$'s represent single-energy-surface conductivity coefficients. The first coefficient in equation (2.8) is the zero-magnetic field electrical conductivity, and the second coefficient is associated with the nondirectional Hall effect. In the limit of weak fields the expansion can be limited to the first two terms. We use the electrical conductivity coefficient, $\sigma_C$, to define the conductivity effective mass $m_{C_i}^*$, by the relationship

$$\sigma_{C_i} = \sigma_{111} = p_i \frac{e^2<\tau_i>}{m_{C_i}^*}$$  \hspace{1cm} (2.9)$$

and the Hall effect coefficient, $\sigma_H$, to define the Hall mobility effective mass by means of [37]

$$\sigma_{H1} = \sigma_{1231} = p_i \frac{e^3<\tau_i^2>}{(m_{H1}^*)^2}$$  \hspace{1cm} (2.10)$$

To solve for $m_{D_i}^*$, $m_{C_i}^*$, and $m_{H1}^*$, equations (2.6), (2.9) and (2.10) are equated to the following expressions for $p_i$, $\sigma_{jk}$, and $\sigma_{jkx}$:

$$p_i = \frac{1}{4\pi^2} \int f_0(k)d^3k$$  \hspace{1cm} (2.11)$$

$$\sigma_{jk} = -\frac{e^2}{4\pi^2\hbar^2} \int \tau \frac{\partial f_0}{\partial E} \frac{\partial E}{\partial k_j} \frac{\partial E}{\partial k_k} d^3k$$  \hspace{1cm} (2.12)$$

$$\sigma_{jkx} = \frac{e^3}{4\pi^2\hbar^4} \int \tau \frac{\partial f_0}{\partial E} \frac{\partial E}{\partial k_j} \frac{\partial E}{\partial k_p} \frac{\partial E}{\partial k_q} \left( \tau \frac{\partial E}{\partial k_k} \right) \epsilon_{kpq} d^3k$$  \hspace{1cm} (2.13)$$
where \( f_0 \) is the Fermi-Dirac distribution function and \( c_{pq} \) is the permutation tensor. Since equations (2.11) through (2.13) do not assume an effective mass, they are valid both for parabolic and nonparabolic band structures. These equations are then evaluated for the model described in Section 2.2.

This procedure yields single \( m_{D1}^*, m_{C1}^*, \) and \( m_{H1}^* \) for an equivalent model which is isotropic and parabolic. These values, in general, will be temperature and carrier-concentration dependent. Although equations (2.6) and (2.11) through (2.13) are expressed in terms of Fermi-Dirac statistics to stress their generality, conductivity and Hall effective masses were derived using Boltzmann statistics to simplify the form of the equation. To obtain values of \( m_{C1}^* \) and \( m_{H1}^* \) we also require a procedure for evaluating \( \langle \tau_i \rangle \) and \( \langle \tau_i^2 \rangle \) in equations (2.9) and (2.10). This will be discussed in Chapter III. The following sections present the expressions for the effective masses in the individual bands.

2.3.1 The Heavy-Hole Band

In this band, the effective masses are given by

\[
m_{D1}^* = \frac{m_0}{(A-B')} \left[ f(-\gamma) \right]^{2/3}
\]

(2.14)

\[
m_{C1}^* = \frac{m_0}{(A-B')} \frac{f(-\gamma)}{f_1(-\gamma)}
\]

(2.15)

and

\[
m_{H1}^* = \frac{m_0}{(A-B')} \left[ \frac{f(-\gamma)}{f_2(-\gamma)} \right]^{1/2}
\]

(2.16)

where \( \gamma \) is defined in equation (2.5). In these equations

\[
f(\gamma) = (1 + 0.05\gamma + 0.01635\gamma^2 + 0.000908\gamma^3 + ...)
\]
\[ f_1(\gamma) = (1 + 0.01667\gamma + 0.041369\gamma^2 + 0.00090679\gamma^3 + 0.00091959\gamma^4 + \ldots) \]

and

\[ f_2(\gamma) = (1 - 0.01667\gamma + 0.017956\gamma^2 - 0.0069857\gamma^3 + 0.0012610\gamma^4 + \ldots) \]

Since the heavy-hole band was assumed parabolic, the integrals containing \( \tau \) in equations (2.9) and (2.10) are identical to those in equations (2.12) and (2.13), and cancel out.

2.3.2 The Light-Hole Band

In the light-hole band, as modeled by Figure 2.1, the effective masses of holes are obtained in terms of partial Fermi-Dirac integrals [25]. Thus

\[
(m^*_{D2})^{3/2} = \frac{2m_0^{3/2}}{\sqrt{\pi}} \left\{ \frac{f(+\gamma)}{(A+B')^{3/2}} \int_0^{\xi/k_0T} \frac{e^{\xi/k_0T}}{\exp(\xi)} \frac{\xi^{3/2}de}{\exp(\xi)} + \right. \\
\left. \frac{f(-\gamma)n_1}{(A-B')^{3/2}} \int_0^{\infty} \frac{\xi^{3/2}de_1}{\exp(\xi_1)} \right\}
\]

(2.17)
\[
m^*_{C2} = \frac{2m_o}{\sqrt{\pi}} \int_0^\infty \frac{\tau \varepsilon^{3/2} \exp(-\varepsilon)}{\varepsilon} \, d\varepsilon \times \left\{ \begin{array}{l}
\frac{f(+\gamma)}{(A+B')^{3/2}} \int_0^{\xi/k_oT} \frac{\varepsilon^{3/2} \exp(-\varepsilon)}{\exp(\varepsilon)} \, d\varepsilon + \frac{f(-\gamma)\eta_1}{(A-B')^{3/2}} \int_0^{\xi/k_oT} \frac{\varepsilon^{3/2} \exp(-\varepsilon)}{\exp(\varepsilon)} \, d\varepsilon \\
\frac{f_1(+\gamma)}{(A+B')^{1/2}} \int_0^{\xi/k_oT} \frac{\tau_2 \varepsilon^{3/2} \exp(-\varepsilon)}{\exp(\varepsilon)} \, d\varepsilon + \frac{f_1(-\gamma)\eta_1}{(A-B')^{1/2}} \int_0^{\xi/k_oT} \frac{\tau_2 \varepsilon^{3/2} \exp(-\varepsilon)}{\exp(\varepsilon)} \, d\varepsilon \end{array} \right\}^{1/2}
\]

\[
m^*_H = m_0 \frac{\tau \varepsilon^{3/2} \exp(-\varepsilon)}{\varepsilon} \left\{ \frac{f(+\gamma)}{(A+B')^{3/2}} \int_0^{\xi/k_oT} \frac{\varepsilon^{3/2} \exp(-\varepsilon)}{\exp(\varepsilon)} \, d\varepsilon + \frac{f(-\gamma)\eta_1}{(A-B')^{3/2}} \int_0^{\xi/k_oT} \frac{\varepsilon^{3/2} \exp(-\varepsilon)}{\exp(\varepsilon)} \, d\varepsilon \right\}^{1/2} \]

(2.19)

where \(\varepsilon_1 = \varepsilon - \Delta/3k_oT\), \(\xi = \xi - \Delta/3\), \(\eta_1 = \exp(-\Delta/3k_oT)\) and \(\Delta\) and \(\xi\) are defined in Figure 2.1.

In this case because equations (2.11) through (2.13) were expressed in terms of partial Fermi-Dirac integrals and equations (2.6), (2.9) and (2.10) were expressed in terms of complete Fermi-Dirac integrals, the dependence on \(\tau\) does not cancel out. Thus the nonparabolicity of the light-hole band introduces a dependence on the scattering relaxation time. The scattering relaxation time is discussed in Chapter III.
2.3.3 The Split-Off Band

Although the split-off band is parabolic, the apparent effective mass in this band will also exhibit a temperature dependence due to the energy displacement at \( k = 0 \). The energy of a hole in the third band is given by

\[
E = E_v - \frac{\pi^2 k^2}{2m_0} A - \Delta
\]  
(2.20)

where \( \Delta \) is the split-off energy (= 0.044eV), and \( A \) is one of the inverse mass band parameters. Substituting equation (2.20) into equations (2.11) through (2.13), and then equating to equations (2.6), (2.9) and (2.10) for the split-off band, we obtain

\[
m_{D3}^* = \frac{m_0}{A} \exp \left( -\frac{2\Delta}{3k_0 T} \right)  
\]  
(2.21)

\[
m_{C3}^* = \frac{m_0}{A} \int_0^\infty \frac{\tau_3 e^{3/2} \exp(-\varepsilon) d\varepsilon}{\int_0^\infty \tau_3 e^{3/2} \exp(-\varepsilon_2) d\varepsilon_2}  
\]  
(2.22)

\[
m_{H3}^* = \frac{m_0}{A} \left[ \int_0^\infty \frac{\tau_3 e^{3/2} \exp(-\varepsilon) d\varepsilon}{\int_0^\infty \tau_3 e^{3/2} \exp(-\varepsilon_2) d\varepsilon_2} \right]^{1/2}  
\]  
(2.23)

where \( \varepsilon_2 = \varepsilon - \Delta/k_0 T \).

The combined hole density-of-state effective mass can be determined by assuming that the total number of holes in the valence band is equal to the sum of the holes in the individual bands
\[ p = p_1 + p_2 + p_3 \] (2.24)

thus

\[ m^*_D = \left[ (m^*_{D1})^{3/2} + (m^*_{D2})^{3/2} + (m^*_{D3})^{3/2} \right]^{2/3} \] (2.25)

This combined effective mass is the mass corresponding to the density-of-states of an effective single equivalent parabolic valence band. This concept is useful in calculations where the effective density-of-states at different temperatures can be calculated from one \( m^*_D \).

The explicit temperature variation of the band curvature is included by assuming that the density-of-states near the band edges varies in a similar manner as the temperature dependence of the energy gap \([25]\). Thus \( (m^*_D)^{3/2} \) is proportional to \( E_{G0}/E_G \) where \( E_{G0} \) is the energy gap at 0 K.

To evaluate the total band equivalent conductivity and Hall effective masses, we assume that in valence band conduction, the total number of holes in motion is equal to the sum of the holes moving on the separate energy surfaces, and that these holes can be modeled as moving on a single spherical energy surface. Thus, the ohmic and the Hall conductivities in the equivalent valence band are given by

\[ \sigma_C = \sigma_{C1} + \sigma_{C2} + \sigma_{C3} \] (2.26)

and

\[ \sigma_H = \sigma_{H1} + \sigma_{H2} + \sigma_{H3} \] (2.27)

respectively.
Substituting equations (2.9) and (2.10) into equations (2.26) and (2.27) it follows that

\[
m^*_{C} = \left\{ \frac{\tau_3}{\tau_1} \left( \frac{\tau_{D1}}{m^*_D} \right)^{3/2} \frac{1}{m^*_C} \frac{\tau_2}{\tau_1} \left( \frac{\tau_{D2}}{m^*_D} \right)^{3/2} \frac{1}{m^*_C} \frac{\tau_3}{\tau_1} \left( \frac{\tau_{D3}}{m^*_D} \right)^{3/2} \frac{1}{m^*_C} \right\}^{-1}
\]

and

\[
m^*_{H} = \left\{ \frac{\tau_1}{\tau_2} \left( \frac{\tau_{D1}}{m^*_D} \right)^{3/2} \frac{1}{m^*_H} \frac{\tau_2}{\tau_2} \left( \frac{\tau_{D2}}{m^*_D} \right)^{3/2} \frac{1}{m^*_H} \frac{\tau_3}{\tau_2} \left( \frac{\tau_{D3}}{m^*_D} \right)^{3/2} \frac{1}{m^*_H} \right\}^{-1/2}
\]

Equations (2.25), (2.28) and (2.29) were evaluated numerically as functions of temperature and acceptor doping density for p-type silicon. Values of the band parameters, $|A| = 4.27$, $|B| = 0.63$ and $|C| = 4.93$, were determined at 4.2 K by Hensel and Feher [22] and Balslev and Lewaetz [29]. In order to simplify the calculations and maintain tractability, anisotropies in the relaxation time were ignored. A rigorous analysis of the conductivities for nonisotropic scattering would be extremely difficult to carry out because no relaxation time is expected to exist in the usual sense [38].

Figure 2.2 shows the dependence of $m^*_D$ with temperature in the range from 100 to 400 K. The slight temperature dependence due to the explicit temperature variation of the curvature at the edge of the band results in an effective mass increase of about five percent in each band at 400 K. This can be seen in the slope of $m^*_D$. The temperature dependence of $m^*_D$ is more pronounced since here we also have the effects of energy displacement at $\overline{k} = 0$. The temperature dependence due to nonparabolicity is very apparent in the shape of the $m^*_D$ curve.
Figure 2.2. Temperature dependence of the density-of-state effective masses $m^*_D$, $m^*_D$, and $m^*_D$, in the individual bands, and the combined density-of-states mass $m^*_D$ of holes in silicon. $N_A = 10^{14}$ cm$^{-3}$. 
The temperature dependence of the conductivity effective mass and the Hall effective mass is shown in Figures 2.3 and 2.4, with the dopant density equal to $10^{14}$ cm$^{-3}$. One consequence of the nonparabolicity of the light-hole band is an increase in the valence band conductivity effective mass as temperature increases from 100 to 400 K. This happens because with increasing thermal energy $k_BT$, more holes reside in the less parabolic regions of the light-hole band. The results plotted in Figure 2.3 show an increase in $m^*_C$ of about 36 percent in this temperature range. The temperature dependence of $m^*_H$ can be attributed mainly to the non-parabolicity of the light-hole band. In the temperature range from 100 to 400 K, $m^*_H$ increases from 0.2850 to 0.5273 $m_0$. The slight temperature dependence of $m^*_C$ and $m^*_H$ is due to the explicit temperature effect and results in increases of 7.7 percent and 3.76 percent in the $m^*_C$ and $m^*_H$ respectively. A larger temperature variation occurs in the case of the split-off band because of the additional effects of the energy displacement at $k = 0$.

Figures 2.5 and 2.6 show the variation of $m^*_C$ and $m^*_H$ with dopant density and temperature. For $T \geq 100$ K, $m^*_C$ varies less than 10 percent in the dopant density range from $10^{14}$ to $10^{18}$ cm$^{-3}$. Since the influence of nonparabolicity is reduced in degenerate material [25], it follows as shown in Figures 2.5 and 2.6 that the variation of effective mass with temperature is much stronger at low dopant densities. At lower temperatures there is a much greater change in effective mass due to variations in scattering relaxation time with percentage of ionized impurities.
Figure 2.3. Temperature dependence of the conductivity effective masses $m_{C1}$, $m_{C2}$, and $m_{C3}$ in the individual bands, and the combined conductivity effective mass $m^*_C$ of holes in silicon. $N_A = 10^{14}$ cm$^{-3}$. 
Figure 2.4. Temperature dependence of the Hall effective masses, $m^*_H$, $m^*_H$, and $m^*_H$, in the individual bands, and the combined Hall effective mass $m^*_H$ of holes in silicon. $N_A = 10^{14}$ cm$^{-3}$. 
Figure 2.5. The acceptor density dependence of the combined conductivity effective mass of holes in silicon as a function of temperature.
Figure 2.6. The acceptor density dependence of the combined Hall effective mass of holes in silicon as a function of temperature.
2.4 Discussion

The idea of temperature-dependent effective mass is supported by a number of experimental data. Cardona et al [21] found an increase of about 12 percent in optical effective mass between 90 and 300 K in heavily-doped p-type silicon. Cyclotron-resonance studies conducted by Hensel and Feher [22] show that when carrier heating populates deeper regions of the light-hole band, the nonparabolic nature of this band at higher values of \( k \) results in an increase in the effective mass of holes.

The model used here in the calculation of hole density-of-states effective mass is identical to that of Barber [25], and consequently our results for \( m^*_D \) and \( m^*_U \) are in excellent agreement with those of Barber [25]. We have extended Barber's work to the calculations of \( m^*_C \) and \( m^*_H \) in p-type silicon. The increase of \( m^*_C \) by 36 percent at 400 K shown in Figure 2.3 is much larger than that reported by Costato and Reggiani (9 percent) [26]. Their calculation was done over a similar range of temperatures, and their value at 100 K, \( m^*_C = 0.342 \ m_o \), is somewhat lower than our calculated value (.3604 \( m_o \)). The discrepancies between our results and those of Costato and Reggiani are due mainly to the correction of \( m^*_U \) for the explicit temperature dependence of the energy gap, the inclusion of the split-off band, and the consideration of unequal relaxation times in the three bands. Note that our calculations of effective masses were achieved through more rigorous mathematical derivations, while those of Costato and Reggiani followed a more empirical curve-fitting type of procedure.

The experimental values of density-of-states effective masses of holes in p-type silicon have been published by numerous authors [21,22, 39,40], but very little data can be found for the conductivity and the
Hall effective masses, making it difficult to properly assess the value of our calculations. There seems to be no obvious way to measure these quantities from d.c. transport measurements. Magneto-kerr effect measurements conducted by Hauge [41], indicate that $m^*$ could increase by as much as 31 percent in the range of temperatures from 100 ($M^*_C = 0.510 M_0$) to 300 K. This is in reasonable agreement with our calculated percentage increase in $m^*_C$ in the same temperature range (33 percent), but it is impossible to compare our calculations with Hauge's experimental results, because our effective mass definition was chosen to be mainly applicable to the study of the Hall and conductivity mobility in the low field limit, and this may not apply to the measurements of Hauge [41].

From the results of this chapter it can be seen that the approximation of a constant effective mass seems to be inadequate to describe transport properties of holes in silicon above 100 K. There is a substantial increase in the effective mass of holes from 100 to 400 K due to the nonparabolicity of the light-hole band, and a smaller, though not negligible, contribution due to the explicit temperature dependence and the effects of the split-off band. The validity of this model for the calculation of density-of-states effective mass has been well established [25]. Barber [25] has shown that when the temperature-dependent effective masses are substituted into the theoretical expression for intrinsic carrier density in silicon, the agreement with reported measurements of $n_i$ is within the limits of experimental error. Application of this model to theoretical calculation of mobility and resistivity in p-type silicon [17] has provided excellent agreement between theoretical and experimental values (resistivity with ±6 percent) over a temperature
range from 100 to 400 K and dopant density range from $10^{14}$ to $3 \times 10^{18}$ cm$^{-3}$. This calculation is limited to applications in conductivity mobility and low field Hall effect.
3.1 Introduction

The study of transport phenomena in semiconductors requires an accurate knowledge of variations in the conductivity mobility and the resistivity with changes in temperature and dopant density. The resistivity is an easily-measured parameter, but the conductivity mobility is a more difficult parameter to evaluate. In general, four different kinds of mobility enter into common discussion [42]. The microscopic mobility is the actual velocity per unit electric field of a free carrier in a crystal. This cannot be measured directly. The conductivity mobility is the mobility associated with the conductivity expression, \( \sigma = e \mu C \). This mobility involves an average relaxation time \( <\tau> \) dependent on the nature of the scattering process, and in the case of nonspherical equal energy surfaces, this mobility also involves a combined effective mass. The Hall mobility is the product of the measured conductivity and the measured Hall coefficient. In general, the Hall mobility differs from the conductivity mobility by a factor called the Hall factor. The drift mobility is the velocity or drift per unit field for a carrier moving in an electric field. If trapping centers are present, so that the actual drift process is not simply motion through the conduction band, but involves a series of trapping and untrapping processes, the drift mobility can be much less than the conductivity mobility. The four mobilities are all equal only when the
following three conditions are met [42]: (a) spherical equal energy surfaces with extremum at $\vec{k} = 0$, (b) relaxation time independent of carrier energy, and (c) negligible trapping effects. Since conditions (a) and (b) are not met in p-type silicon, it is improper to judge the behaviour of one kind of mobility based on knowledge of a different kind of mobility. Thus drift or Hall mobility data cannot be tacitly assumed to be accurate substitutes for conductivity mobility values.

As mentioned above, the conductivity mobility involves an average scattering relaxation time. In any semiconductor, the charge carriers (i.e., holes and electrons), at temperatures above absolute zero, may be scattered by a number of mechanisms. Different mechanisms are dominant in certain temperature and dopant density regimes, but in some cases two or more may be interacting simultaneously. Thus in calculating the conductivity mobility over a wide range of temperatures and dopant densities, all the relevant scattering mechanisms must be taken into account. In the case of silicon, acoustic and optical phonon scattering, and ionized and neutral impurity scattering are of major importance. Hole-hole scattering also plays an important role in determining the mobility. In the following sections the theoretical effects of these scattering mechanisms on the mobility will be considered.

3.2 Mobility and Average Scattering Relaxation Time

The calculation of mobility of holes in the valence band of silicon is accomplished by evaluating the mobility separately in the heavy-hole band, the light-hole band, and the split-off band considering all appropriate scattering mechanisms. The overall mobility is then evaluated as a weighted average of the single-band mobilities over the individual hole densities in each band.
The conductivity mobility in each of the three valence bands is calculated from

\[ \nu_{Ci} = \frac{e^{<\tau_i>}}{m_i^*} \tag{3.1} \]

where

\[ <\tau_i> = \frac{\int \varepsilon^{3/2} \tau_i \left( \frac{\partial f_0}{\partial \varepsilon} \right) d\varepsilon}{\int \varepsilon^{3/2} \left( \frac{\partial f_0}{\partial \varepsilon} \right) d\varepsilon} \tag{3.2} \]

for the case of Fermi-Dirac statistics, and \( \tau_i \) represents the total scattering relaxation time in band \( i \). Because each scattering mechanism has its own dependence on scattering energy, a simple closed form expression for total scattering relaxation time as a function of temperature cannot be obtained. The use of numerical techniques is necessary to solve for the relaxation time. In the case of p-type silicon, the peculiarities of a degenerate, warped, and nonparabolic valence band must be taken into account [1]. The possibility of interband as well as intraband transitions must also be taken into account in the analysis. With the inclusion of interband scattering as given by Bir et al. [43], the total relaxation time in the heavy- \( (i = 1) \) and light-holes \( (i = 2) \) bands is given by

\[ \tau_i = \frac{1}{\delta} \left( 1 + \frac{m_i^*}{m_j^*} \frac{\tau_{ij}}{\tau_{ii}} \right) \tau_{ii} \quad i \neq j; \quad i = 1, 2; \quad j = 1, 2 \tag{3.3} \]

where
\[ \delta = 1 - \frac{T_{11} T_{22}}{T_{12} T_{21}} \]  

(3.4)

and

\[ \tau_{ii} = \left[ \tau_{aci}^{-1} + \tau_{oi}^{-1} + \tau_{li}^{-1} + \tau_{Ni}^{-1} \right]^{-1} \]  

(3.5)

The total relaxation time in the split-off band is given by

\[ \tau_3 = \left[ \tau_{ac3}^{-1} + \tau_{o3}^{-1} + \tau_{i3}^{-1} + \tau_{N3}^{-1} \right]^{-1} \]  

(3.6)

Only transitions between the light- and heavy-hole band are considered; the relaxation time \( \tau_{ji} \) takes into account a transition from band \( i \) to band \( j \); and \( \tau_{aci} \), \( \tau_{oi} \), \( \tau_{li} \), and \( \tau_{Ni} \) are the relaxation times corresponding to scattering by acoustical phonons, optical phonons, ionized impurities, and neutral impurities respectively, with \( i \) as the band index. The procedure for including the nonparabolicity of the band structure into calculations of relaxation time, consists of modifying the relaxation time for a given scattering process by replacing the temperature independent effective mass of the parabolic band by the temperature dependent effective mass of the nonparabolic band. This procedure has been successfully applied to the study of acoustic phonon scattering in nonparabolic bands by Radcliffe [18]. Optical phonon and ionized impurity scattering in nonparabolic bands have been considered by Barrie [19] in the same manner. Braggins [1] has used the same method to include nonparabolicity in his study of p-type silicon. In this work, the relaxation times appropriate to degenerate, parabolic valence bands have been used and modified according to the prescription of Radcliffe [18], Barrie [19], and Braggins [1]. The
anisotropy of the energy spectrum is not considered in this model, because from the transport theory for parabolic bands it is known that this anisotropy has no influence on the temperature dependence of mobility, but only on its absolute value [10]. Each of the four scattering mechanisms will now be discussed.

3.3 Acoustical Phonon Scattering

The relaxation time for scattering by acoustical phonons includes both the possibility of interband as well as intraband scattering. The treatment of the acoustical phonons has been based on the theory of Bir, Normantas, and Pikus [43] where the relaxation times can be expressed in terms of a single constant, \( \tau_x \), which controls the overall magnitude of the scattering. Both transverse and longitudinal phonons participate in the scattering so that

\[
\tau_{acl}^{-1} = \frac{m^*_{ACL}}{\tau_x} \left\{ L_{11}^{(2)} + \gamma_{ij}^3 L_{11}^{(1)} + \right. \\
\left. \frac{C_e^2}{C_t^2} \beta^2 \left[ T_{11}^{(2)} + \gamma_{ij}^3 T_{11}^{(1)} \right] \right\} \tau^{3/2} \epsilon^{1/2} \tag{3.7}
\]

and

\[
\tau_{acl}^{-1} = \frac{m^*_{ACL}}{\tau_x} \left\{ L_{22}^{(2)} + \gamma_{ij}^3 L_{22}^{(1)} + \right. \\
\left. \frac{C_e^2}{C_t^2} \beta^2 \left[ T_{22}^{(2)} + \gamma_{ij}^3 T_{22}^{(1)} \right] \right\} \tau^{3/2} \epsilon^{1/2} \tag{3.8}
\]
for intraband scattering, while

\[ \tau_{ij}^{-1} \gamma_{ij}^{-5} = \tau_{ji}^{-1} = \frac{m^*_{Di}}{\tau_x} \left\{ L_{ij}(2) + \right. \]

\[ \frac{C_L^2}{C_t^2} \beta^2 \tau_{ij}(2) \right\} \tau^{3/2} \epsilon^{1/2} \]

(3.9)

for interband scattering. In the split-off band, the scattering relaxation time is given by

\[ \tau_{\text{ac}3}^{-1} = \frac{1}{\tau_x} \left( \epsilon - \frac{\Delta}{k_0 T} \right)^{1/2} T^{3/2} \]

(3.10)

In these equations

\[ \frac{1}{\tau_x} = \frac{k_o^{3/2} a^2 m_o^{3/2}}{\sqrt{2\pi} \hbar \rho_s c^2} \]

(3.11)

\[ \gamma_{ij} = \frac{m^*_{Di}}{m^*_{Dj}}, \quad \beta = b/a, \quad a \text{ and } b \text{ are valence band acoustic deformation potential constants in the Picus and Bir [44] notation, } \rho_s \text{ is the density, } C_L \text{ and } C_t \text{ are the longitudinal and transverse sound velocities in silicon and } L_{ij} \text{ and } T_{ij} \text{ are functions of } \beta \text{ and } \gamma_{ij} \text{ defined in [43].} \]

3.4 Optical Phonon Scattering

Optical phonon scattering, while negligible at very low temperatures, cannot be ignored at high temperatures. Ehrenreich and Overhauser [45] have calculated the mobility of holes in silicon and its dependence on temperature. The calculated mobility follows a $T^{-2.3}$ dependence for reasonable choices of the parameters which described the
mixing of optical and acoustical phonon scattering. This agrees with experimental results \[5,8\]. The relaxation time for scattering by nonpolar optical phonons is given by [46]

\[
\tau_{0i}^{-1} = \frac{m^*_{Di}}{\tau_x} W_0 D^{-1/2} \left\{ \left(n_0 + 1\right) \left(\epsilon - \frac{\theta_D}{T}\right)^{1/2} + n_0 \left(\epsilon + \frac{\theta_D}{T}\right)^{1/2} \right\}
\]

where \(\theta_D\) is the Debye temperature, \(n_0 = (\exp(\theta_D/T)-1)^{-1}\) is the phonon distribution function, and \(W\) is a constant which determines the relative coupling strength of the holes to the optical phonon mode compared to the acoustical phonon mode.

\[
W = \frac{D_0^2 \hbar^2 c^2}{2 k_0^2 a^2 \theta_D^2}
\]

where \(D_0^2\) is the optical deformation potential constant. The first term in the brackets of equation (3.12) corresponds to optical phonon emission and is relevant only when this is energetically possible \((\epsilon > \theta_D/T)\). The second term in the brackets corresponds to optical phonon absorption.

### 3.5 Ionized Impurity Scattering

The Coulomb interaction between ionized impurities and charge carriers drifting through the crystal under the action of an applied electric field causes scattering of the charge carriers. Scattering by ionized impurities was first considered by Conwell and Weisskopf [47]. The basic assumption is that the Coulomb field is cut off at half the
distance between charged impurities. This is equivalent to assuming that a charge carrier sees only one charged impurity at a time, the effect of the other charged impurities being sufficiently screened as to be negligible. This approach was improved by Brooks [48] and Herring [49] who associated the cut-off of the Coulomb potential with a screening distance, the free carriers being assumed to provide screening against the charge of the impurities. In the low dopant density limit, the scattering relaxation time due to ionized impurities is given by [48,49]

\[ \tau_{II}^{-1} = \frac{\pi e^4 N_A G(b_i)}{(2m_{Di}^* \frac{1}{2} \epsilon_s^2 (k_0 T)^{3/2}}\epsilon^{-3/2}, \quad i = 1, 2, 3 \quad (3.14) \]

where

\[ G(b_i) = \ln(b_i+1) - \frac{1}{(b_i+1)} \quad (3.15) \]

and

\[ b_i = \frac{24\pi m_{Di}^* \epsilon_s (k_0 T)^2}{e^2 \hbar^2 p'} \quad (3.16) \]

where \( p' \) is the screening carrier density, \( p' = p + N_A(1 - N_A/N_D) \), for \( N_D = 0 \).

3.6 Neutral Impurity Scattering

Scattering by neutral impurities in semiconductors has been considered by Erginsoy [50] as a variation of the problem of the scattering of electrons by neutral hydrogen atoms. The result is a temperature independent relaxation time given by
where $N_N$ is the density of neutral impurities and $m^*_{G}$ is the geometric mean mass appropriate for evaluating the scaled Bohr radius term [48]. Sclar [51,52] has included the possibility of bound states in the evaluation of electron-hydrogen impurity scattering by using a three-dimensional square well to estimate the influence of a weakly-bound state on the scattering. In this case the relaxation time is given by

$$\tau_{N_1}^{-1} = \left( \frac{\varepsilon_{s} m^2_{e}}{m^*_{G} \varepsilon^2} \right) \frac{20 \pi^2}{m^*_{D1}} N_N, \quad i = 1, 2, 3 \quad (3.17)$$

$E_1$ is the binding energy of neutral acceptors.

For silicon doped with shallow impurities, this type of scattering is important at low temperatures where neutral impurities may outnumber ionized impurities. For the deeper levels, where neutral impurities can exist at higher temperatures, the influence of neutral impurity scattering can extend over a wide range of temperatures.

3.7 Effect of Hole-Hole Scattering

The expressions thus far presented for scattering relaxation time neglect the effect of hole-hole scattering. Although hole-hole scattering does not affect the current density directly since it cannot alter the total momentum, it tends to randomize the way in which this total
momentum is distributed among holes of different energies. When the scattering mechanism is such as to lead to a nonuniform distribution, hole-hole scattering gives rise to a net transfer of momentum from holes which dissipate momentum less efficiently to those which dissipate momentum more efficiently, resulting in an overall greater rate of momentum transfer, and lower mobility [53]. Thus the size of the effect of hole-hole scattering on the scattering relaxation time is a function of the energy dependence of the relaxation time. The hole-hole reduction factor, \( \gamma_{hh} \), can be derived by means of a classical formulation introduced by Keyes [54]. When hole-hole collisions are much more frequent than hole-acceptor collisions, the average relaxation time for a parabolic band in the Keyes [54] approximation approaches the limiting form

\[
\langle \tau_{hh} \rangle = \frac{\int \epsilon^{3/2} \left( \frac{3f_0}{\epsilon} \right) d\epsilon}{\int \epsilon^{3/2 - 1} \left( \frac{3f_0}{\epsilon} \right) d\epsilon}
\]

(3.20)

where \( f_0 \) is the Fermi-Dirac distribution function. On the other hand, if hole-hole collisions are neglected, the average relaxation time is given by equation (3.2).

Thus the hole-hole reduction factor (i.e., the ratio of \( \langle \tau_{hh} \rangle \) to \( \langle \tau \rangle \)) can be expressed as

\[
\gamma_{hh} = \left\{ \frac{\int \epsilon^{3/2} \frac{3f_0}{\epsilon} d\epsilon \times \int \epsilon^{3/2 - 1} \frac{3f_0}{\epsilon} d\epsilon}{\int \epsilon^{3/2} \left( \frac{3f_0}{\epsilon} \right)^2 d\epsilon} \right\}^{-1}
\]

(3.21)
\[
Y_{hh} = \frac{-1}{<\tau><\tau^{-1}>} \quad (3.21a)
\]

for optical phonon scattering, and \(Y_{hh}^0\), the hole-hole reduction factor, is evaluated from equation (3.21).

For acoustical phonon scattering it is assumed that \(Y_{hh}^a\) decreases linearly with increasing dopant density from a value of one to a value 
\[Y_{hh}^a = \frac{9\pi}{32} = 0.88 \quad (17)\]
in a certain range of impurity concentration. The exact relationship \(Y_{hh}^a = 1.0004 - 4.013378 \times 10^{-19}N_A, 10^{15} \leq N_A \leq 3 \times 10^{17}\) is determined empirically with a best fit of the experimental data.

Luong and Shaw [55] using a one-particle-like approximation from the Hartree-Fock theory, have shown that by inclusion of hole-hole scattering, the Brooks-Herring [48,49] formula is reduced by a factor which can be expressed in closed form as

\[
Y_{hh}^i = \left(\frac{N_A}{p^s}\right) \left[1 - \exp\left(p^s/N_A\right)\right] \quad (3.22)
\]

where \(N_A\) is the ionized acceptor density and \(p^s\) is the screening hole density. In the case of neutral impurity scattering, hole-hole scattering has no significance because \(\tau_N\) is independent of hole energy.

Thus the overall scattering relaxation time in each hole band is calculated from equations (3.3), (3.5), and (3.6) with the terms of these equations properly corrected for the effects of hole-hole scattering. Because the individual energy surfaces are different from each other, the relaxation times also differ from each other and cannot be assumed equal except in restricted ranges of temperature and dopant density [43].
3.8 Mobility in the Combined Valence Band

The conductivity mobility in each individual band is calculated from equation (3.1), and the combined conductivity mobility in the valence band is then evaluated as a weighted average of the single-band mobilities over the population of holes in each band, thus

\[ \mu_C = \mu_1 \left( \frac{m^*_1}{m^*_D} \right)^{3/2} + \mu_2 \left( \frac{m^*_2}{m^*_D} \right)^{3/2} + \mu_3 \left( \frac{m^*_3}{m^*_D} \right)^{3/2} \] (3.23)

Using equation (3.23) and the parameters listed in Table 3-1, we have calculated the hole mobility for silicon doped with boron, gallium, and indium as functions of dopant density and temperature, for \( 10^{14} \leq N_A \leq 10^{18} \text{cm}^{-3} \) and \( 100 \leq T \leq 400 \text{ K} \). The results are displayed in Figures 3.1 through 3.6. In the calculations of mobility and resistivity in silicon doped with gallium and indium, it was assumed that boron impurities were also present. Since very pure silicon has a resistivity on the order of \( 1000\Omega\text{-cm} \), it was assumed that boron densities of \( 10^{13} \) and \( 5 \times 10^{13} \text{cm}^{-3} \) existed in the gallium- and indium-doped samples, respectively. The values of these background densities were deduced from a best fit of the experimental data. For this reason, especially in the case of indium-doped silicon, the actual role of the impurities at low temperatures and/or low dopant densities is masked by the action of the always present boron impurities. As the dopant density and temperature increase, the assumed background densities of boron impurities become insignificant compared to the density of ionized dopant atoms, and Figures 3.1 through 3.6 accurately depict the influence of the particular type of impurity on the resistivity and mobility of holes in p-type silicon. The figures also show that for the case of the
Table 3-1. Values used in the calculations.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
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<td>$\Delta$</td>
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</tr>
<tr>
<td>$a$</td>
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<td>eV</td>
</tr>
<tr>
<td>$b$</td>
<td>-1.36*</td>
<td>eV</td>
</tr>
<tr>
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<td></td>
</tr>
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<td>$\Theta_D$</td>
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<td>K</td>
</tr>
<tr>
<td>$\rho_s$</td>
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<td>kg/m$^3$</td>
</tr>
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<td>$\varepsilon_0$</td>
</tr>
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<td></td>
</tr>
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<td>kg</td>
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<tr>
<td>$k_0$</td>
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<td>joules/K</td>
</tr>
<tr>
<td>$e$</td>
<td>$1.6 \times 10^{-19}$</td>
<td>coul</td>
</tr>
</tbody>
</table>

* These values were obtained from references [1] and [22].
Figure 3.1. The calculated hole mobility vs dopant density for boron-doped silicon with temperature as a parameter.
Figure 3.2. The calculated hole mobility vs dopant density for gallium-doped silicon with temperature as a parameter.
Figure 3.3. The calculated hole mobility vs dopant density for indium-doped silicon with temperature as a parameter.
Figure 3.4. The calculated hole mobility vs temperature for boron-doped silicon with dopant density as a parameter.
Figure 3.5. The calculated hole mobility vs temperature for gallium-doped silicon with dopant density as a parameter.
Figure 3.6. The calculated hole mobility vs temperature for indium-doped silicon with dopant density as a parameter.
shallower ionization energies, the mobility depends more strongly on temperature for the lightly-doped case where lattice scattering is dominant and become less temperature dependent as the dopant density increases.

The constant, $\tau_x$, was found by fitting the mobility to experimental data in the lattice-scattering-limited range. Our value of $\tau_x$ is equivalent to an acoustic deformation potential constant of 8.099 eV. The optical phonon coupling constant, $W$, was then found by fitting the mobility to the high temperature experimental data. Our value of $W$ is equivalent to an optical deformation potential constant of $6.024 \times 10^8$ eV/cm.
CHAPTER IV
HOLE DENSITY AND RESISTIVITY

4.1 Introduction

The resistivity of semiconductor materials is one of their most useful and easily measured properties. Theoretical calculations of resistivity depend on the formulation of conductivity mobility, and the determination of hole density. For extrinsic semiconductors, the hole density is determined primarily by the percentage of ionization of impurity atoms. The following sections discuss the dependence of hole density and resistivity on temperature and dopant density.

4.2 Ionization of Impurity Atoms

For the case of Fermi-Dirac statistics, the hole density is given by

\[ p = \frac{4}{\sqrt{\pi}} \left( \frac{2\pi k T m^*}{h^2} \right)^{3/2} \frac{F_{3/2}(\eta)}{n} \]  

(4.1)

where, \( m^* \), the density-of-states effective mass, contains information pertaining to the nonparabolic nature of the valence band. In the limit of low dopant densities, equation (4.1) reduces to

\[ p = N_v \exp(\eta) \]  

(4.2)

where \( N_v = 2(2 \pi m^* k T/\hbar^2)^{3/2} \) is the effective density of valence band states. For the range of temperatures considered in this study, the
hole density is calculated by assuming that the density of carriers is determined by the impurities present in the silicon sample. The density of ionized acceptor impurities in p-type silicon is computed from the charge neutrality equation

\[ N_A - N_D = p - n \] (4.3)

This reduces to

\[ p = N_A \] (4.4)

for the case of uncompensated material.

The density of ionized acceptors is [56]

\[ N_A = \frac{N_A}{1 + g \exp \left( \frac{E_A - E_F}{k_B T} \right)} \] (4.5)

where \( E_A \) is the acceptor ionization energy, and \( g \) is the ground state degeneracy. Excited states have a very minor influence on the carrier concentration due to the large separation between the ground state and the excited states [1,56]. Letting

\[ g = 4 + 2 \exp \left( - \frac{\Delta}{k_B T} \right) \] (4.6)

enables us to include the contribution of the split-off band [17]. The density of ionized acceptors is computed by iterating \( E_F \) in equations (4.2) and (4.5) until equation (4.4) is fulfilled within a given level of accuracy.
Experimental evidence shows that the acceptor ionization energy $E_A$ is not a constant, but decreases with increasing dopant density [9]. Penin et al. [57] have determined in a study of heavily doped silicon from 4 to 300 K that for shallow impurities such as boron and phosphorus the ionization energy decreases and finally disappears altogether for impurity densities greater than $3 \times 10^{18}$ cm$^{-3}$. For impurities with deeper activation energies, it is also expected that at some impurity concentration, the impurity activation energy should become a function of the impurity concentration. However, in the case of gallium and indium, this should happen at higher impurity concentrations than for the shallower level impurities. This is due to the smaller geometrical dimensions of the wave functions applicable to the deeper levels, so that overlapping effects which promote the reduction in activation energy require higher impurity concentrations [14]. For shallow impurities such as boron and phosphorus, empirical expressions [9,57] relating the dependence of ionization energy to dopant density have been established. In the case of Ga, there is data [15] on activation energy vs concentration, but not enough on which to base an accurate relationship. For this reason the value of $E_A = 0.056$eV was used. For In, $E_A = 0.156$eV [58] was used. Figures 4.1 through 4.3 show the ratio of ionized and total impurity density as a function of impurity density with temperature as a parameter for $100 \leq T \leq 400$ K for silicon doped with boron, gallium, and indium. It is clearly shown in these figures that the ionization of impurities for the deeper levels is significantly lower even at low dopant densities so that it is necessary to go to higher
Figure 4.1. Theoretical calculations of the ratio of ionized and total boron density vs boron density with temperature as a parameter.
Figure 4.2. Theoretical calculations of the ratio of ionized and total gallium density vs gallium density with temperature as a parameter.
Figure 4.3. Theoretical calculations of the ratio of ionized and total indium density vs indium density with temperature as a parameter.
temperatures to achieve total ionization of impurities. The deionization of impurities is most significant for low temperatures and high impurity densities.

4.3 Resistivity of p-Type Silicon

The resistivity of p-type silicon is given by

\[ \rho = \frac{1}{\mu C \rho} \]  

where \( \mu \) is the hole conductivity mobility calculated from equation (3.23) and \( \rho \) is the hole density discussed in Section 4.2. Equation (4.7) was used to calculate the hole resistivity for silicon doped with boron, gallium, and indium as a function of dopant density and temperature, for \( 10^{14} \leq N_A \leq 10^{18} \text{ cm}^{-3} \) and \( 100 \leq T \leq 400 \text{ K} \). The results are displayed in Figures 4.4 through 4.9. In the calculations of resistivity in silicon doped with gallium and indium, as was done for conductivity mobility, it was assumed that boron impurities were also present. Boron densities of \( 10^{13} \) and \( 5 \times 10^{13} \text{ cm}^{-3} \) were assumed to exist in the gallium- and indium-doped samples, respectively. The values of these background densities were deduced from a best fit of the experimental data. As the dopant density and temperature increase, the assumed background densities of shallow impurities becomes insignificant compared to the density of ionized dopant atoms, and Figures 4.4 through 4.9 accurately depict the influence of the particular type of impurity on the resistivity of holes in p-type silicon. The figures also show that for the case of the shallower ionization energies, resistivity depends more strongly on temperature for the lightly doped case where lattice scattering is dominant and become less temperature dependent as the dopant density increases.
Figure 4.4. Theoretical calculations of resistivity vs temperature for boron-doped silicon with dopant density as a parameter.
Figure 4.5. Theoretical calculations of resistivity vs temperature for gallium-doped silicon with dopant density as a parameter.
Figure 4.6. Theoretical calculations of resistivity vs temperature for indium-doped silicon with dopant density as a parameter.
Figure 4.7. Theoretical calculations of resistivity vs dopant density for boron-doped silicon with temperature as a parameter.
Figure 4.8. Theoretical calculations of resistivity vs dopant density for gallium-doped silicon with temperature as a parameter.
Figure 4.9. Theoretical calculations of resistivity vs dopant density for indium-doped silicon with temperature as a parameter.
5.1 Introduction

The most direct determination of the mobility is by the Haynes-Schokley drift method, wherein the drift of charge carriers in a known electric field is measured. However, the assumption, made when these experiments were initiated, that the drift mobility of holes as minority carriers in an n-type sample is the same as when they constitute the majority carriers, is invalid in view of carrier-carrier scattering [59]. Also the experiment can succeed only if the lifetime of the minority carriers is larger than the transit time. For this reason, usually Hall mobilities are measured instead. The Hall mobility is the product of the measured conductivity and the measured Hall coefficient. In general the Hall mobility differs from the conductivity mobility by a factor called the Hall factor. Determination of the Hall factor may be avoided by making use of the high field limit. For sufficiently high magnetic fields several simplifications occur in the magnetic field dependence of the Hall coefficient. In the high-field limit (when the product of mobility and magnetic induction becomes greater than $10^8 \text{ cm}^{-2} \text{ gauss/volt-sec}$ [60]) the Hall coefficient is simply related to the carrier concentration by [61]

$$R_H = \frac{1}{pe} \quad (5.1)$$
and thus the conductivity mobility and the Hall mobility are equal. Although the high field limit simplifies use of the Hall mobility considerably, excessively high magnetic fields can cause problems due to the quantization of the hole orbits in a magnetic field [1]. The quantization of the particle motion in a magnetic field will create Landau levels within the band. The Landau levels will modify the density of states in the valence band which could affect the interpretation of experimental data [56]. Another high magnetic field effect of importance is the "magnetic freeze out" which occurs with the stronger localization of bound state wave-functions in a strong magnetic field [62]. Due to the more localized charge distribution, the Coulomb binding energy of the impurity state is increased so that at a fixed temperature the concentration of thermally excited charge carriers will be smaller and the Hall coefficient will be effectively increased.

Thus, in order to avoid these high field region complications and obtain an experimental determination of the value of conductivity mobility in the low field limit, it is necessary to have an accurate knowledge of the Hall factor with which to modify measured Hall mobilities. Hall measurements are routinely used to experimentally determine the density of ionized impurities in a semiconductor sample. This determination is possible only if an accurate value of the Hall factor for the particular temperature and dopant density considered is available.

5.2 **The Hall Factor**

The Hall and conductivity mobilities are related by the Hall factor as follows:
For nondegenerate, spherically symmetric bands, it can be shown that
\[ r_H = \frac{\mu_H}{\mu_C} \]  
(5.2)

and that
\[ r_H = \frac{<\tau^2>}{<\tau>^2} \]  
(5.3)

In general most previous work \([5,59]\) has assumed that equation (5.3) is valid in the case of p-type silicon and thus \( r_H \) will vary between 1.18 \((\tau(E) \propto E^{-1/2} \) for lattice scattering\) and 1.93 \((\tau(E) \propto E^{3/2} \) for ionized impurity scattering\), if hole-hole scattering is neglected, and will approach unity for the degenerate case. This theory does not allow for values of \( r_H \) less than one. Experimental evidence indicating values of \( r_H \) less than one has been attributed to poor quality of the measured samples \([5]\). Debye and Kohane \([63]\) found that the measured drift mobility for holes is considerably larger than the measured Hall mobility. Values of \( r_H \) less than unity were also reported by Wolfstirn \([15]\) for the case of gallium-doped silicon. More recent experiments \([64]\) show that a value of \( r_H \) less than unity is necessary to reconcile differences between the hole concentration measured via Hall coefficient methods and that inferred from dopant densities determined from C-V and junction breakdown measurements. The usual assumption made is to let \( r_H \) be equal to one and thus consider the Hall mobility equal to the conductivity mobility. Neglecting the Hall scattering factor alters both the magnitude and temperature dependence of the carrier concentration from that given by the charge balance equation. In fitting data to the charge balance equation, both thermal
carrier concentration and dopant impurity activation energy are overestimated by the assumption of unity Hall factor. A more complete theoretical treatment of the Hall factor can be undertaken by considering the nonparabolic and anisotropic nature of the valence band of silicon.

Chapter II described the constant energy surfaces as warped spheres. Warping of the energy surfaces has a significant effect on the ratio of Hall to conductivity mobility. When the bands are warped, the Hall factor depends on the degree of warping as well as the scattering mechanism [30].

The Hall mobility is the product of the ohmic conductivity and the Hall coefficient

$$\mu_H = \sigma_C R_H$$

(5.4)

In the low field limit the Hall coefficient for a nonparabolic, anisotropic band $i$ is given by [37]

$$R_{Hi} = \frac{\sigma_{Hi}}{\sigma_{Ci}}$$

(5.5)

Thus by substituting equations (2.9) and (2.10) into equation (5.5) the Hall coefficient can be expressed as

$$R_{Hi} = \frac{r_{Hi}}{p_i e}$$

(5.6)

where
is the Hall factor. We see that allowing for a difference between the values of conductivity and Hall effective masses due to the anisotropic, nonparabolic nature of the band, enables us to separate the Hall factor into two components: the mass anisotropy factor given by

\[ r_{Ai} = \frac{\left\langle T_1 \right\rangle^2}{m_c^* m_{Hi}^*} \]  

(5.8)

and the scattering factor given by

\[ r_{Si} = \frac{\left\langle T_1 \right\rangle^2}{\left\langle \tau_1 \right\rangle^2} \]  

(5.9)

These components of the Hall factor will be considered in detail in the next two sections.

5.3 The Mass Anisotropy Factor

Lax and Mavroides [20] have derived expressions for \( r_A \) based on the Dresselhaus et al [28] model of the valence band of germanium and silicon. Their formulation for \( r_A \) acknowledges the anisotropy, but neglects the nonparabolicity of the bands. In general it is found that \( r_A \) is less than unity unless the scattering anisotropy becomes extreme [30]. In order to determine the variation of the mass anisotropy factor with changes in temperature and dopant density for the combined valence band of silicon, equation (5.8) was evaluated using the values of combined valence band effective mass obtained from equations (2.28) and (2.29).
The results of this calculation are presented in Figures 5.1 and 5.2. These figures show the significant contribution of the mass anisotropy factor to the Hall factor. Since the influence of nonparabolicity is reduced in degenerate material [25], it follows as shown in Figures 5.1 and 5.2, that the variation of $r_A$ with temperature is much stronger at low dopant densities, since it is in this dopant density range that the variation of effective mass with temperature is the strongest. We note that the mass anisotropy factor is less than unity for all temperatures considered in this work once the dopant density increases past $6 \times 10^{15}$ cm$^{-3}$. At 300 K, $r_A$ is less than unity even for dopant densities as low as $10^{14}$ cm$^{-3}$.

5.4 The Scattering Factor

The scattering factor, $r_S$, depicted in Figures 5.3 and 5.4 as a function of temperature and dopant density, does not follow the traditionally expected variation between $3\pi/8 = 1.18$ and $315\pi/512 = 1.93$ as the dominant scattering mechanism changes from lattice to ionized impurity scattering. Putley [65] has noted that hole-hole scattering can modify $r_S$. He estimates that for ionized impurity scattering, $r_S$ can be reduced from $315\pi/512$ to a value close to unity. At low dopant densities where the dominant scattering mechanism is acoustic phonon scattering, $r_S$ varies between 1.08 for $T = 100$, to 1.24 for $T = 400$ K. The deviation from the traditionally expected value of $r_S = 1.18$ is due to the contributions of optical phonon modes at the higher temperatures. Hole-hole collisions also affect the impurity and optical phonon scattering contributions so they become significant even at low temperatures and dopant densities. At higher values of dopant density, the effects of hole-hole scattering on the ionized impurity scattering mechanism
Figure 5.1. The mass anisotropy factor $r_A$ as a function of temperature for various impurity dopant densities.
Figure 5.2. The mass anisotropy factor $r_A$ as a function of impurity dopant density for various temperatures.
Figure 5.3. The scattering factor $r_s$ as a function of temperature for boron-doped silicon with dopant density as a parameter.
Figure 5.4. The scattering factor $r_s$ as a function of dopant density for boron-doped silicon with temperature as a parameter.
THE MOBILITY, RESISTIVITY AND CARRIER DENSITY IN P-TYPE SILICON--ETC(U)

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become very noticeable. At \( N_A = 10^{18} \text{ cm}^{-3} \), the highest value of \( r_5 \) is 1.29 for \( T = 100 \text{ K} \), where the dopant impurities are only about 30 percent ionized [17]. At higher temperatures where the percentage of ionized impurity atoms is over 80 percent, the effects of hole-hole scattering bring \( r_5 \) from its traditionally expected value of 1.93 to 1.05 for \( T = 400 \text{ K} \).

5.5 Hall Mobility and Hall Factor in the Combined Valence Band

Expressions for Hall coefficient, applicable in the case where holes in more than one band take place in conduction, are given by Putley [66]. For the case of p-type silicon, assuming no compensation and operation in the low field region, the Hall coefficient is given by [66]

\[
R_H = \frac{\sum_{i=1}^{3} R_{Hi}^2 \sigma_{Ci}^2}{\left( \sum_{i=1}^{3} \sigma_{Ci} \right)^2} \tag{5.10}
\]

By substituting equations (2.9) and (5.6) through (5.10) into equation (5.4), the Hall mobility in the combined valence band of silicon can be expressed by

\[
\mu_H = e \left\{ \frac{3}{\sum_{i=1}^{3} \frac{m^*_{Di}}{m^*_{Hi}} \langle \tau_i \rangle^{3/2}} \right\}
\tag{5.11}
\]
The conductivity mobility for the combined valence band can be expressed by

\[ \mu_C = \frac{e}{m_D^{3/2}} \left\{ \sum_{i=1}^{3} \frac{m_i^{*3/2}}{m_i^{*} \langle \tau_i \rangle} \right\} \tag{5.12} \]

Then using equations (5.11) and (5.12) we can express the Hall factor in terms of the scattering relocation times and effective masses of the individual bands by

\[ r_H = \frac{3}{\sum_{i=1}^{3} \frac{m_i^{*3/2}}{m_i^{*} \langle \tau_i \rangle}^{2}} \tag{5.13} \]

Figures 5.5 and 5.6 summarize the results of equation (5.13) as a function of temperature and dopant density. These figures show that the Hall factor ranges theoretically between 1.73 and 0.77 for temperatures between 100 and 400 K and dopant densities between \(10^{14}\) and \(10^{18}\) cm\(^{-3}\). For temperatures above 200 K, \(r_H\) becomes less than unity for dopant densities greater than \(5.5 \times 10^{15}\) cm\(^{-3}\). Figures 5.7 and 5.8 show the theoretically predicted Hall mobility as functions of temperature and dopant density. These two figures show the results of evaluating equation (5.11) with the aid of numerical integration, and adjusting the lattice scattering mobility to give the best fit to values of conductivity mobility deduced from resistivity measurements.
Figure 5.5. Theoretical Hall factor vs temperature for boron-doped silicon with dopant density as a parameter.
Figure 5.6. Theoretical Hall factor vs dopant density for boron-doped silicon with temperature as a parameter.
Figure 5.7. Theoretical Hall mobility as a function of temperature for boron-doped silicon with dopant density as a parameter.
Figure 5.8. Theoretical Hall mobility as a function of dopant density for boron-doped silicon with temperature as a parameter.
6.1 Introduction

Experimental measurements of resistivity, Hall coefficient and dopant density were made on six silicon wafers, four doped with gallium, and two doped with indium, in dopant densities ranging from $4.25 \times 10^{15}$ to $3.46 \times 10^{17}$ cm$^{-3}$. These wafers were cut from crystals grown along the $<111>$ and $<100>$ direction. Additional data were obtained from boron-doped silicon wafers to further verify the adequacy of the theory. The data were obtained from test patterns NBS-4 [67] fabricated on the silicon wafers. This test pattern was designed at the National Bureau of Standards primarily for use in the evaluation of the resistivity versus dopant density relation in silicon. Resistivity measurements were made on four-probe square array resistors and collector Hall effect resistors, while the net dopant density in the specimens was determined by the junction C-V method on a gated base-collector diode. Mean values of resistivity, dopant density and Hall coefficient were determined by measuring five to eight selected test cells with a standard deviation in resistivity at 300 K under five percent. The following sections describe the test sample preparation and fabrication procedure, and the measurement procedures.
6.2 Fabrication Procedure

The overall pattern is fabricated on a square silicon chip 200 mils on a side where six mask levels are used [68]. The masks were used in the following sequence: base, emitter, base contact, gate oxide, contact and metal. Appropriate cleaning procedures (see Appendix A) precede the diffusion of impurities, and a negative photoresist process was used in the masking steps. The base mask delineates regions whose conductivity type is opposite from that of the collector substrate, and the emitter mask delineates regions whose conductivity type is the same as that of the collector substrate. A base region approximately two \( \mu \text{m} \) deep is diffused into the background material; then the emitter region is diffused into the base to a depth of approximately one \( \mu \text{m} \). The base contact mask is used to open windows onto the base region, where an \( n^+ \) diffusion is made to improve ohmic contact to the base. The gate oxide mask delineates regions where an oxide layer of closely controlled thickness is grown to serve as a gate for MOS devices. After front-side metallization, a portion of the wafer was separated. This section was scribed to provide the Hall effect devices. The remainder of the wafer was then metallized on the backside and alloyed. After scribing, the devices were mounted on TO-5 headers, metal contact bonding was made, and the devices were encapsulated. A layer of ceramic insulating material was used to isolate the devices from contact with the header. Resistivity measurements were then made to select devices for use in this study.
6.3 Experimental Measurements

The structures used to evaluate the resistivity of the bulk material are the Hall effect resistor and the collector four-probe resistor [68]. The four-probe resistor has four point contacts arranged in a square array. The structure (see Appendix A) is fabricated by diffusing a base over a large area except at the four point contacts which are protected from the base diffusion by oxide islands. Emitters are diffused at these points in order to make low resistance contacts to the collector material. The purpose of the base diffusion is to eliminate surface currents. The bulk resistivity is determined by forcing a current, I, between two adjacent probes and measuring the voltage, V, between the other two probes. The resistivity of the material is determined from [69]

\[ \rho = \frac{2\pi SV}{(2-\sqrt{2})IC'} \quad (6.1) \]

where \( S \) is the probe spacing and \( C' \) is a correction factor dependent on the ratio of probe spacing to the thickness of the chip [70]. This correction factor is given by

\[ C' = 1 + \frac{4}{2-\sqrt{2}} \sum_{n=1}^{\infty} (-1)^n \left[ 1 + \frac{4n^2w^2}{S^2} \right]^{-1/2} - \frac{2\sqrt{2}}{2-\sqrt{2}} \sum_{n=1}^{\infty} (-1)^n \left[ 1 + \frac{2n^2w^2}{S^2} \right]^{-1/2} \quad (6.2) \]

where \( w \) is the thickness of the chip.

The collector Hall effect resistor is a four-terminal resistor formed in a square chip 100 mils on a side. Contacts are formed on the
four corners by an emitter diffusion (see Appendix A). The resistivity is calculated from [71]

\[ \rho = \frac{\pi w}{2n^2} \frac{V}{I} \]  

(6.3)

where \( w \) is the thickness of the chip, and \( V \) is the voltage difference between nearest neighbor contacts for a current, \( I \), passed between the remaining two contacts. The TO-5 header was mounted in the sample holder of an Air Products and Chemicals AC-3L CRYO-TIP liquid nitrogen system. This enabled variation of the sample temperature between 100 and 350 K. The temperature was measured by a chromel vs gold with 0.07 atomic percent iron thermocouple. For temperatures above 350 K, the sample was placed in a Stratham Temperature Test Chamber.

The structure used for the Hall coefficient measurements is the collector Hall effect resistor. The Hall coefficient is calculated from

\[ R_H = \frac{V_Hw}{BI} \]  

(6.4)

where \( V_H \) is the voltage difference measured between opposite contacts for a current, \( I \), passed between the remaining two contacts, and \( B \) is the magnetic field density perpendicular to the plane of the chip; thus the samples are oriented so that the magnetic field is in the crystal growth direction, \(<111>\) for the gallium-doped samples, and \(<100>\) for the indium-doped samples. The Hall mobility is determined from
\[ \nu_H = \frac{R_H}{\rho} \]  

(6.5)

where \( \rho \) is determined from resistivity measurements on the Hall and four-point structures. The magnetic field for the Hall measurements was provided by a Varian Associates (V3703) six-inch electromagnet with a current regulated power supply (V-FR2503). The magnetic field strength was monitored by a Bell 620 gaussmeter with an STB4-0402 probe with a stated accuracy of 0.1 percent. Data was taken over a temperature range from 100 to 350 K. The current used in the resistivity and Hall coefficient measurements was provided by a Keithley 225 current source capable of accuracy within ±0.5 percent of the three-digit readout. The current was monitored by voltage readings across precision resistors connected in series with the current source. These resistors were part of a Dana-651 current shunt set, accurate to within 0.01 percent. Voltages were measured with a Hewlett Packard 3465A digital multimeter with a stated accuracy within 0.03 percent of the readout. Resistivity and Hall coefficient measurements were made in accordance with ASTM standard procedures [72].

The impurity dopant density was obtained by use of two different structures: an MOS capacitor, and a base-collector diode. The MOS capacitor over collector consists of a main gate which is surrounded by a field plate that overlaps a channel stop which also serves as top side collector contact [68]. This structure (see Appendix A) is used to measure the collector dopant density \( (N_A + N_D) \) from the high frequency C-V deep depletion method [73]. The collector dopant density is determined by obtaining a dopant profile from C-V measurements by means of
\[ N(x) = \frac{2}{e \varepsilon A^2} \frac{\Delta V}{\Delta C^2} \]  

(6.6)

where \( \Delta V \) is an incremental change in the gate voltage, and the measured capacitance is due to both the oxide and the semiconductor. A self-consistent check was made on the measurements of collector dopant density by using the base-collector diode. This structure (see Appendix A) consists of a base diffused into a collector and a metal field plate to control the periphery. The field plate overlaps both the base and a diffused emitter channel stop which also serves as topside collector \[68\]. To obtain a correct density profile the field plate is biased at the flat-band potential \[74\]. Capacitance-voltage measurements were taken with a Princeton Applied Research 410 C-V Plotter and a Hewlett Packard 7010A X-Y Recorder.

From each silicon wafer, eight four-probe resistors, eight Hall resistors, and eight capacitor-diode chips were selected for encapsulation. These were chosen on the basis of low leakage currents and good contacts at the metal bonding pads. Measurements were made on each of the devices and data from the five to eight devices closest to the mean value of the measurements were then averaged. In this manner we arrived at representative values of resistivity, Hall coefficient, and dopant density for each sample. The results of these measurements and comparisons with the theory of Chapters III through V are presented in the next chapter.
CHAPTER VII
COMPARISON OF THEORETICAL AND EXPERIMENTAL RESULTS

7.1 Conductivity Mobility

Conductivity mobility was evaluated by substituting the measured resistivities into equation (4.7). Figure 7.1 shows the hole mobility plotted as a function of hole density at 300 K for boron-doped silicon. Curve 1 represents the theoretical results of equation (3.23), and curve 2 was reproduced from the work of Wagner [8]. Our calculated values are within six percent of the values reported by Wagner for $N_A \leq 3 \times 10^{17}$ cm$^{-3}$. For higher values of hole density our calculated values are substantially higher than those of Wagner. As previously explained by Li [17], this discrepancy is due to Wagner's assumption of complete ionization of boron impurities. This assumption is valid only at low dopant densities or at high temperatures where full ionization of boron atoms prevails. The theoretical calculation is in excellent agreement (within three percent) with experimental data reported by Thurber et al [12]. This gives support to the validity of ionization calculations based on equations (4.2) through (4.6).

Mobility values reported by Horn [13] are also in reasonable agreement with our theoretical results. The data points shown in Figure 7.1 were corrected for deionization effects via equations (4.2) through (4.6).
Figure 7.1. Hole mobility vs hole density for boron-doped silicon at 300 K. Curve 1 is the theoretical calculation from equation (3.23), and curve 2 is reproduced from Wagner [8]. Shown also are the experimental results of this work, Horn [13], and Thurber et al [12]. All data points have been corrected for deionization effects.
7.2 Resistivity

The resistivity vs dopant density relationship for boron-doped silicon at 300 K is shown in Figure 7.2. The solid line represents theoretical calculations using equation (4.7). Wagner's [8] resistivity curve and the theoretical line coincide over most of the boron density range. Our theoretical calculations agree with Wagner's resistivity data within six percent over the entire range of boron densities considered at T = 300 K. Excellent agreement exists between our experimental data and the theoretical calculations at 300 K. Figure 7.2 also shows excellent agreement between our theoretical calculations and the data of Thurber et al [12]. Good agreement was obtained with the data of Thurber and Carpenter [75] where total boron density was obtained by the nuclear track technique.

Figure 7.3 shows the resistivity of gallium- and indium-doped silicon as a function of total dopant density for T = 300 K. As expected, because of the deeper ionization energy of indium as compared to gallium, values of resistivity for gallium doped silicon are lower than values of resistivity for indium-doped silicon at the same total dopant density. Figure 7.3 does not show this at low dopant densities because of the assumed values of background boron impurity densities. Excellent agreement was obtained between our experimental data and that obtained from Wolfstirn [15] for gallium-doped silicon, and our theoretical calculations at T = 300 K. Data obtained from the two indium-doped samples showed good agreement with the theoretical calculations, but the same was not true for the data of Schroder et al [64], and Backenstoss [16]. As seen in Figure 7.3, for each value of measured resistivity, Schroder et al [64] report two different values of measured indium density. The
Figure 7.2. Resistivity vs dopant density for boron-doped silicon at 300 K. Shown are the theoretical calculations from equation (4.7) and the experimental results of this work, Thurber and Carpenter [75], and Thurber et al [12].
Figure 7.3. Resistivity vs dopant density for gallium- and indium-doped silicon at 300 K. Shown are theoretical calculations from equation (4.7) and the experimental results of this work, Wolfstirn [15], Schroder et al [64], and Backenstoss [16].
lower value of indium density was obtained by C-V and junction breakdown methods, while the higher value was obtained by Hall measurements and curve fitting. Because of uncertainties in the value of the Hall scattering factor, Schroder et al consider the lower value of density more reliable. Note that our theoretical calculation falls between the two values of dopant density reported by Schroder et al [64]. Values of resistivity of indium-doped silicon reported by Backenstoss [16] are about 25 percent higher than our calculated values. The work of Backenstoss [16], however, was done in the high doping region where dopant densities approach the limit of solid solubility. Backenstoss found that for dopant densities greater than $4 \times 10^{17}$ cm$^{-3}$ there was a considerable amount of indium precipitation. Thus it is possible that part of the discrepancy between our theoretical calculations and the data of Backenstoss is due to the low solid solubility limit of indium in silicon. Recent theoretical results of Sclar [14] for In-doped silicon also agree very closely with our theoretical calculations at 300 K.

To find out the adequacy of our theoretical model for temperatures other than 300 K, we compared the calculated and measured values of resistivity for silicon samples doped with boron, gallium and indium for temperatures ranging from 100 to 400 K. Figure 7.4 shows the comparison between the theoretical and measured resistivities for boron-doped silicon. Except for a couple of data points, agreement between the theoretical and measured values was within 8 percent over the entire range of temperatures. Figures 7.5 and 7.6 show the comparison between theoretical and measured resistivities for gallium- and indium-doped silicon respectively. Agreement here was not as good as in the boron-doped case, but except for a couple of data points, agreement between
Figure 7.4. Resistivity vs temperature for the boron-doped silicon samples. Solid lines are the theoretical calculations and solid dots are the experimental data.
Figure 7.5. Resistivity vs temperature for the gallium-doped silicon samples. Solid lines are the theoretical calculations and solid dots are the experimental data.
Indium-Doped Silicon

Figure 7.6. Resistivity vs temperature for the indium-doped silicon samples.
theory and experiment was within 10 percent. For the indium-doped samples, the largest discrepancies occurred at low temperatures. This is suggestive of some degree of compensation in the samples. An experimental estimate of percentage of compensation was not made for any of the silicon samples studied in this work.

7.3 Hall Mobility

Figures 7.7 through 7.12 show the experimentally determined Hall mobility for silicon slices doped with gallium and indium. Agreement between theory and experiment is good for temperatures above 150 K for the gallium-doped samples. However, for temperatures of 150 K and below some points differ from the theoretical prediction by as much as 38 percent. The measured Hall mobility of the indium-doped samples is well within 15 percent of the calculated value except for one data point at $T = 100$ K. Our control over the temperature of the samples was better for the $T = 200$ K range, but the main source of the discrepancy between theoretical and experimental values of Hall mobility is the Hall factor. This will be discussed in the next section. The magnetic field was rated accurate to within 1 percent. Data points representing a Hall mobility-dopant density pair are estimated to have a total error of around 8 percent.

7.4 Hall Factor

The Hall factor in the case of p-type silicon, is plotted as a function of dopant density for $T = 300$ K in Figure 7.13. With the exception of the points deduced from Morin and Maita's [5] data for boron-doped silicon, agreement between the Hall factor-dopant density data and the theoretical calculation is within 15 percent for
Figure 7.7. Hall mobility vs temperature for gallium-doped sample. 
\(N_A = 4.25 \times 10^{15} \text{ cm}^{-3}\).
Figure 7.8. Hall mobility vs temperature for gallium-doped sample. 

\( N_A = 4.09 \times 10^{16} \text{ cm}^{-3} \).
Figure 7.9. Hall mobility vs temperature for gallium-doped sample. 
$N_A = 1.26 \times 10^{17}$ cm$^{-3}$. 

Gallium-Doped Silicon 

$N_A = 1.26 \times 10^{17}$ cm$^{-3}$
Figure 7.10. Hall mobility vs temperature for gallium-doped sample. 

\[ N_A = 3.46 \times 10^{17} \text{ cm}^{-3} \]
Figure 7.11. Hall mobility vs temperature for indium-doped sample.

\[ N_A = 4.64 \times 10^{16} \text{ cm}^{-3} \]
Figure 7.12. Hall mobility vs temperature for indium-doped sample.

\[ N_A = 6.44 \times 10^{16} \text{ cm}^{-3} \]
Figure 7.13. Hall factor vs dopant density for p-type silicon at 300 K. Shown are the theoretical calculations from equation (5.13) and the experimental results of this work, Wolfstirn [15], Morin and Maita [5], and Schroder et al [64].
$N_A > 5 \times 10^{15}$ cm$^{-3}$. While in general, agreement between theory and experiment in this region of dopant density is only within 15 percent, the bulk of the experimental data is within 10 percent of the theoretical prediction. The samples used by Morin and Maita [5] showed a considerable degree of compensation; in their lower-doped samples, the compensation was as high as 20 percent. This fact may have contributed to the low values of measured Hall mobility, and the large discrepancy between these data points and the calculation. This model neglects the effects of compensation, and the combined presence of acceptor impurities of varying ionization energies. The overall effect of adding impurities of both signs is one of increased ionization of the excess $N_A$ or $N_D$ [15]. It would be necessary to know the percentages of compensation of the experimentally measured crystals to accurately determine the adequacy of the theory at low dopant densities. An experimental estimate of percentage of compensation was not made for any of the silicon samples studied in this work. Long [38] has noted that the low measurements of Hall mobility for p-type silicon may not be due entirely to compensation and the quality of the crystals. For reasonably pure silicon samples ($\rho = 35$ ohm-cm, $N_A = 4.4 \times 10^{15}$ cm$^{-3}$) Long [33] obtained Hall mobilities between 360 and 390 cm$^2$/volt-sec. Hall mobilities as great as 450 cm$^2$/volt-sec have also been reported [76]. While higher than the Hall mobilities of Morin and Maita, these measurements [38, 76] still indicate a value of Hall factor for low-doped p-type silicon at 300 K less than unity. It is still doubtful that a Hall mobility smaller than a conductivity mobility at 300 K is really an intrinsic property of p-type silicon [38]. It is possible that the Hall factor may be greater than unity in a crystal of exceptionally high perfection. However, calcu-
lations involving an exact model of the valence band of silicon [77] indicate that the anisotropy of the bands, while not important in the interpretation of mobility and resistivity data, plays an important role in the evaluation of the Hall factor. Our model averages out the anisotropy of the bands and thus our values of the mass anisotropy factor, $r_A$, are larger than an exact model would predict. A calculation based on the exact model, applicable over the entire range of interest of temperatures and dopant densities, is beyond the scope of this work. At the higher dopant densities there is fair agreement between the theoretical prediction and values of Hall factor deduced from our experimental work and the data of Wolfstirn [15]. Data points from Wolfstirn's work showing ionization energies greater than 0.065 eV were not included in Figure 7.13 because of the high degree of compensation of these samples.
CHAPTER VIII
SUMMARY AND CONCLUSIONS

Theoretical expressions have been derived to compute the hole mobility, resistivity and Hall factor as functions of dopant density and temperature for silicon doped with boron, gallium and indium. The valence band of silicon was represented by a three-band model which takes into account the nonparabolic nature of the bands. This attribute of the valence band is included in the effective mass calculations. Contributions from scattering by acoustical and optical phonons, ionized impurities and neutral impurities were considered in the calculation of average relaxation time. In addition, our model also takes into account the effect of hole-hole scattering on both lattice and ionized impurity scattering relaxation times, and the effect of inter-band transitions on the acoustic phonon relaxation time. Thus the model developed in this study represents a more complete theoretical description of the conductivity mobility, Hall mobility, Hall factor and resistivity than previous theoretical models have acknowledged.

As stated in Chapter II, the model used for the valence band of silicon provides values of density-of-states effective mass which lead to values of intrinsic carrier density which are well within the limits of experimental error. The greatest deficiency this model has over an exact calculation is that the anisotropy of the bands has been averaged out. Thus while the temperature dependence of effective mass derived from the exact and approximate models of the valence band is similar,
the magnitudes of the masses may be substantially different. This difference is not relevant in the study of mobility and resistivity in p-type silicon, but becomes important in the determination of the Hall factor. Since direct experimental verification of values of conductivity and Hall effective masses is not possible, the only way to assess the value of effective mass calculations is by using the theory in the development of directly measurable properties such as resistivity and Hall mobility.

The resistivity analysis for the boron-, gallium-, and indium-doped silicon samples showed agreement between experimental and theoretical results within 10 percent over the entire range of temperature, $100 \leq T \leq 400$ K. Note that best agreement between theory and experiment was obtained for boron-doped samples, followed by gallium- and indium-doped samples. This may be due to the fact that we neglect the compensation effect and the possible dependence of ionization energy on dopant density in the theoretical calculations for gallium- and indium-doped samples. An experimental estimate of degree of compensation was not made for any of the silicon samples studied here. Data points representing a resistivity-dopant density pair are estimated to have a total error of around 6 percent.

A comparison between our calculated mobility values with those of Wagner's [8] data on boron-doped silicon at 300 K shows that agreement is within ±6 percent for $N_A \leq 3 \times 10^{17}$ cm$^{-3}$. Discrepancies at higher dopant densities can be eliminated if the effect of deionization of boron impurities were included in Wagner's calculations [8]. Excellent agreement was found between our theoretical calculations of mobility in boron-doped silicon and the data of Thurber et al [12] at 300 K. We
have obtained excellent agreement between theoretical values of resistivity and our experimental data for boron-, gallium-, and indium-doped silicon at 300 K; our theoretical calculations also agreed with the resistivity data by Thurber et al [12] for boron-doped silicon, and Wolfstirn [15] for gallium-doped silicon.

As shown in Chapter V, however, this theoretical model does not have the same kind of success in describing the Hall mobility and Hall factor for p-type silicon for low dopant densities, and low temperatures. For dopant densities lower than $5 \times 10^{16}$ cm$^{-3}$, this model predicts a value of Hall factor much greater than has been experimentally determined [5,15,38]. A discrepancy like this for the case of p-type germanium was eliminated as the quality of germanium crystals improved. Thus it has been assumed that low values of Hall mobility for low-doped p-type germanium at $T = 300$ K were caused by compensation. However, compensation alone may not account for low values of Hall mobility in the case of p-type silicon [38]. Recent studies by Nakagawa and Zukotynski [77] indicate that the use of the exact model in the development of the Hall factor formulation yields results which agree in general with experimental data for the case of p-type silicon. Experimental data for the case of p-type germanium does not agree with the theoretical results of Nakagawa and Zukotynski [77].

From this study, we have found that the theoretical expressions derived in this work are adequate for mobility and resistivity calculations for p-type silicon in the temperature range $100 \leq T \leq 400$ K, and the dopant density range $10^{14} \leq N_A \leq 10^{18}$ cm$^{-3}$. The theoretical formulation is also adequate for description of the Hall factor and Hall mobility for dopant densities above $5 \times 10^{16}$ cm$^{-3}$ and temperatures above
200 K. The failure of this model in predicting Hall factor and Hall mobility at low temperatures and dopant densities is due to the omission of the proper anisotropy formulation in the model of the valence band of silicon. This weakness in the model would be remedied by use of the exact model in a manner similar to that of Nakagawa and Zukotynski [11,77].

Further improvements to this model would include the exact formulation of the valence band of silicon on Kane's [27] model, as prescribed by Nakagawa and Zukotynski [11,77]. Thus the proper nonparabolicity and anisotropy would be included. For better comparison with experimental results, the variation of ionization energy with dopant density should be included in the calculation of hole density for the deeper impurities. Also the effects of compensation and the presence of other p-type impurities in silicon samples must be considered. It would also be of great benefit to extend this study into the heavy doped region.
APPENDIX A

FABRICATION PROCEDURES AND TEST STRUCTURES

This appendix contains a list of the fabrication procedures followed to generate the test structures measured in this study. These test structures were part of NBS-4 [67] test pattern, and include a planar four-probe collector resistor, a 100 mil square Hall effect device, a gated base-collector diode, and a gated MOS capacitor over collector structure.

A.1 Initial SiO₂ Masking:

A.1a Initial Clean Up:

1. Ultrasonic clean in hot DI water with small amount of 100 Tritonex solution for 10 minutes.
2. Rinse in running DI water for 5 minutes.
3. Place in solution of 1NH₄OH:1H₂O₂:2H₂O for 20 minutes at 50 degrees C.
4. Rinse in DI water for 5 minutes.
5. Dip in 10 percent HF for 10 seconds.
6. Rinse in DI water for 5 minutes.
7. Place in solution of 1HCl:1H₂O₂:2H₂O for 20 minutes at 50 degrees C.
8. Rinse in DI water for 10 minutes and spin dry in N₂.

A.1b Initial Oxidation - 350 nm at 1100 degrees C

1. Push-in 5 minutes N₂ at 1000 cc/minute
(2) Dry $O_2$ 5 minutes $O_2$ at 800 cc/minute
(3) Wet $O_2$ 35 minutes $O_2$ at 800 cc/minute
(4) Dry $O_2$ 5 minutes $O_2$ at 800 cc/minute
(5) $N_2$ 15 minutes $N_2$ at 1000 cc/minute
(6) Pull-out 5 minutes $N_2$ at 1000 cc/minute

A.2 Phosphorus Base Diffusion:

A.2a Photoresist (PR) Application with Base Mask (NBS-4-1AB):

(1) Bake at 200 degrees C for 30 minutes to completely dry the wafer.

(2) Apply Waycoat 200 negative PR (do this on both sides of the wafer, apply and spin PR on back side first).

(3) Spin at 5000 RPM for 20 seconds.

(4) Prebake in 65-degree C oven for 20 minutes.

(5) Align wafer and mask and expose for 4 seconds under UV light. (Both sides of the wafer must be exposed.)

(6) Develop for 20 seconds in spray of Waycoat developer (undiluted), then clean off developer with 15-second spray of Butyl Acetate.

(7) Dry with $N_2$ and inspect under the microscope.

(8) Post bake at 130 degrees C for 25 minutes in $N_2$ or air circulating oven.

A.2b Base Window Etch:

(1) Etch in buffered HF for 2 minutes, rinse in DI water, dry and inspect. Etch for 15 seconds more to see if the pattern changes color.
(2) When certain that all the oxide has been removed, place
wafer in hot (90 degrees C) J-100 PR remover for 5
minutes.
(3) Quench/rinse in methanol for 5 minutes, then rinse with
methanol from squirt bottle.
(4) Rinse in DI water for 5 minutes.
(5) Clean up - same as above A.1a except for ultrasonic
clean.

A.2c Phosphorus Base Diffusion at 875 degrees C:
(1) Push-in 5 minutes $N_2$ at 1250 cc/minute
(2) Phosphorus 16 minutes $N_2$ at 1250 cc/minute
$O_2$ at 100 cc/minute
$N_2$ through source
bubbler at 10 cc/
minute
$T$(source) = 4 to 7
degrees C
(3) Flush-out 2 minutes $O_2$ at 800 cc/minute
$N_2$ at 1250 cc/minute
(4) Pull-out 5 minutes $N_2$ at 1250 cc/minute

A.2d Removal of Phosphosilicate Glass:
(1) Dip in 10 percent HF for 5 seconds.
(2) Rinse in DI water for 5 minutes and spin dry in $N_2$.

A.2e Drive-in Diffusion and Base Oxide - 350 nm at 1100 degrees C,
base depth approximately 2um:
(1) Push-in 5 minutes $N_2$ at 1000 cc/minute
(2) Dry $O_2$ 10 minutes $O_2$ at 800 cc/minute
(3) Wet $O_2$ 45 minutes $O_2$ at 800 cc/minute
(4) Dry $O_2$ 10 minutes $O_2$ at 800 cc/minute
(5) Drive-in 70 minutes $N_2$ at 1000 cc/minute

A.3 Boron Emitter Diffusion:
A.3a PR with Emitter Mask NBS-4-2AB - Same as A.2a (front side PR only), with the following change: Before applying Waycoat PR, coat surface of the wafer with silazane (5 parts Hexamethyldisilazane: 95 parts Xylene), and spin at 4000 RPM for 20 seconds.
A.3b Emitter Window Etch:
(1) Etch in buffered HF for 2.5 minutes, rinse in DI water, dry and inspect. Etch for 15 seconds more to see if the pattern changes color.
(2) When certain that all oxide has been removed (oxide islands must be gone), strip PR and clean up same as A.2b (5).
A.3c Boron Nitride Diffusion at 1050 degrees C:
(1) Load wafers facing source.
(2) Push-in 5 minutes $N_2$ at 500 cc/minute
(3) Pre-dep 30 minutes $N_2$ at 500 cc/minute $O_2$ at 25 cc/minute
(4) Oxide 10 minutes $O_2$ at 1000 cc/minute
(5) Pull-out 5 minutes $N_2$ at 500 cc/minute
A.3d Removal of Borosilicate Glass:
(1) Dip in 10 percent HF for 10 seconds.
(2) Rinse in DI water for 5 minutes, spin dry in $N_2$. 
A.3e Boron Drive-in and Emitter Oxide, $T = 925$ degrees C:

1. Push-in 5 minutes $N_2$ at 1000 cc/minute
2. Dry $O_2$ 5 minutes $O_2$ at 1000 cc/minute
3. Wet $O_2$ 65 minutes $O_2$ at 1000 cc/minute
4. Dry $O_2$ 5 minutes $O_2$ at 1000 cc/minute
5. Passivation 5 minutes $N_2$ at 1000 cc/minute
6. Pull-out 5 minutes

A.4 Base Contact Diffusion:

A.4a PR with Contact Diffusion Mask NBS-4-5AB - Same as A.2a (PR on both sides - back side first). Back side must be exposed.

A.4b Base Contact Window Etch:

1. Etch in buffered HF for 2 minutes, 45 seconds. Rinse dry, check for oxide removal.
2. When all oxide has been removed strip PR and clean up same as A.2b (5).

A.4c Phosphorus Base Contact Diffusion at 875 degrees C:

1. Push-in 5 minutes $N_2$ at 1250 cc/minute
2. Pre-dep 10 minutes $N_2$ at 1250 cc/minute $O_2$ at 100 cc/minute $N_2$ through source bubbler at 10 cc/minute $T$(source) = 4 to 7 degrees C
3. Flush-out 2 minutes $O_2$ at 800 cc/minute
4. Pull-out 5 minutes $N_2$ at 1250 cc/minute
A.4d Removal of Phosphosilicate Glass:

(1) Dip in 10 percent HF for 5 seconds.
(2) Rinse in DI water for 5 minutes and spin dry in N₂.

A.4e Reoxidation at 95 degrees C:

(1) Push-in 5 minutes N₂ at 1000 cc/minute
(2) Dry O₂ 10 minutes O₂ at 1000 cc/minute
(3) Wet O₂ 25 minutes O₂ at 1000 cc/minute
(4) Dry O₂ 5 minutes O₂ at 1000 cc/minute
(5) Passivation 5 minutes N₂ at 1000 cc/minute
(6) Pull-out 5 minutes

A.5 MOS Gate Oxide:

A.5a PR with Gate Oxide Mask NBS-4-6AB - Same as A.2a (PR on front side only, use silizane).

A.5b Etch in Buffered HF for 3 minutes, rinse, dry and check for oxide removal.

A.5c When all oxide has been removed strip PR and clean up same as A.2b (5).

A.5d Gate Oxide Growth - 12000Å at 950 degrees C:

(1) Push-in 5 minutes N₂ at 1000 cc/minute
(2) Dry O₂ 10 minutes O₂ at 800 cc/minute
(3) Wet O₂ 40 minutes O₂ at 800 cc/minute
(4) Dry O₂ 10 minutes O₂ at 800 cc/minute
(5) Passivation 10 minutes N₂ at 1000 cc/minute
(6) Pull-out 5 minutes

A.6 Contact Windows:

A.6a PR with Contact Mask NBS-4-3AB. Same as A.2a (front side only, use silizane).
A.6b Contact Window Etch:
   (1) Etch in buffered HF for 3 minutes, check for complete removal of oxide.
   (2) Strip PR and clean up same as A.2b.

A.7 Front Side Metallization:
   A.7a In the alloy furnace set at 450 degrees C, 5 minutes in N$_2$;
       15 minutes in forming gas, 5 minutes in N$_2$. Gas flow = 800 cc/minute in all cases.
   A.7b Evaporate 800 nm aluminum over the front surface of the wafer.
   A.7c PR with Metal Mask NBS-4-4AB. Same as A.2a (front side only, use silizane).
   A.7d Etch in Al etchant of 20 H$_3$PO$_4$:5H$_2$O:1HN heated to 50 degrees C until the etching is complete (about 2 minutes).
   A.7e Rinse in DI water for 10 minutes.
   A.7f Strip PR in J-100 and methyl as prescribed in A.2b (3 minutes in 80 degrees C J-100).

A.8 Back Side Contact:
   A.8a Dry for 30 minutes in 200-degree C oven.
   A.8b Spin PR on front side as prescribed in A.2a (no mask).
       Expose to U.V. light for 4 seconds.
   A.8c Hard bake at 130 degrees C for 30 minutes.
   A.8d Dip in 10 percent HF until oxide has been removed from the backside of the wafer.
   A.8e Remove PR in J-100 and methyl as prescribed in A.2b (do not use cleaning procedure).
   A.8f Scribe the wafer to separate the Hall devices.
A.8g Evaporate 400 nm aluminum over the back side of chips.

A.9 Post Evaporation Micro Alloy. Load chips in alloy furnace at 500 degrees C for 15 minutes. \( \text{N}_2 \) set for a flow rate of approximately 100 cc/minute.
Figure A.1. Square array collector resistor. Pipe size = 0.40x0.40 mil, \( S = 2.25 \text{ mil (57.15 \text{ \(\mu\text{m})}, t = 4.75 \text{ mil (121 \text{ \(\mu\text{m})}, NBS - 4.7 \[67].}
Figure A.2. Hall effect device. NBS - 4.31 [67].
Figure A.3. Gated base-collector diode. Diameter = 17 mils (431.8 μm).
NBS - 4.8 [67].
Figure A.4. Gated MOS capacitor over collector. Diameter = 15 mils (381 μm), NBS = 4.8 [67].
APPENDIX B
EXPERIMENTAL SETUP AND DATA

This appendix consists of a block diagram which shows the experimental setup and equipment used, and six tables which show the data taken on the test structures. In addition to measured values of resistivity, dopant density and Hall coefficient, Tables B-1 through B-6 also contain values of calculated Hall mobility.
Figure B.1. Experimental Set-up. For Hall effect measurements the magnetic field was generated by a Varian Associates 6 in. Electromagnet System #544772. Capacitance measurements were taken with a Princeton Applied Research-410 C-V Plotter #601922 and a HP-7010A X-Y Recorder #602659.
Table B-1. Sample SGA 16-2 (Ga-Doped Si, $N_A = 4.25 \times 10^{15}$ cm$^{-3}$)

<table>
<thead>
<tr>
<th>Temperature ($T$) (K)</th>
<th>Resistivity ($\rho$-cm)</th>
<th>Hall Coefficient ($R_H$ cm$^3$/coulomb)</th>
<th>Hall Mobility ($\mu_H$ cm$^2$/v-sec)</th>
</tr>
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<tbody>
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Table B-2. Sample SGA 16-3 (Ga-Doped Si, $N_A = 4.09 \times 10^{16}$ cm$^{-3}$)

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<th>Resistivity $\rho$(Ω-cm)</th>
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Table B-3. Sample SGA 17-2 (Ga-Doped Si, $N_A = 1.26 \times 10^{17} \text{ cm}^{-3}$)

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<th>Temperature T(K)</th>
<th>Resistivity $\rho$(Ω-cm)</th>
<th>Hall Coefficient $R_H$(cm$^3$/coulomb)</th>
<th>Hall Mobility $\mu_H$(cm$^2$/v-sec)</th>
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Table B-4. Sample SGA 18-2 (Ga-Doped Si, \( N_A = 3.46 \times 10^{17} \text{ cm}^{-3} \))

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<th>Hall Coefficient (R_H (\text{cm}^3/\text{coulomb}))</th>
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Table B-5. Sample SIN 16-2 (In-Doped Si, $N_A = 4.64 \times 10^{16} \text{ cm}^{-3}$)

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<th>Resistivity ($\Omega$-cm)</th>
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Table B-6. Sample SIN 17-1 (In-Doped Si, $N_A = 6.44 \times 10^{16}$ cm$^{-3}$)

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<th>Temperature $T$(K)</th>
<th>Resistivity $\rho$(Ω-cm)</th>
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<th>Hall Mobility $\mu_H$(cm$^2$/v-sec)</th>
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</thead>
<tbody>
<tr>
<td>100</td>
<td>25.95</td>
<td>58958</td>
<td>2272</td>
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<tr>
<td>150</td>
<td>4.65</td>
<td>7268</td>
<td>1563</td>
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<tr>
<td>200</td>
<td>1.564</td>
<td>1345</td>
<td>860</td>
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<tr>
<td>250</td>
<td>0.952</td>
<td>458</td>
<td>481</td>
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<tr>
<td>300</td>
<td>0.766</td>
<td>237</td>
<td>309</td>
</tr>
<tr>
<td>350</td>
<td>0.721</td>
<td>158</td>
<td>219</td>
</tr>
<tr>
<td>400</td>
<td>0.740</td>
<td></td>
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</tbody>
</table>
APPENDIX C
COMPUTER PROGRAM

This appendix contains the FORTRAN computer program used to generate values of conductivity and Hall effective mass, conductivity and Hall mobility, and Hall factor as functions of temperature and acceptor impurity density in silicon. Besides the main program, two subroutines are also listed. The first of these, DENSTY, calculates the hole density by iterating the Fermi energy level in the charge balance equation as explained in Chapter IV; the second, INTBND, computes the coefficients (functions $L_{ij}$ and $T_{ij}$ of equations (3.7) through (3.9)) used in the calculations of acoustic phonon scattering based on the work of Bir et al [43].
10C CONDUCTIVITY EFFECTIVE MASS, HALL EFFECTIVE MASS,
20C CONDUCTIVITY MOBILITY, HALL MOBILITY, AND
30C HALL FACTOR AS FUNCTIONS OF TEMPERATURE AND
40C ACCEPTOR IMPURITY DENSITY IN SILICON
50C DOPED WITH BORON
60C
70 REAL MD1,MD2,MD3,MD,NN,NAI,NA,LI,MI
80 REAL M1,M2,M3,M1T,M2T,M3T,K,K0,M0,KT
90 REAL MH,MH1,MH2,MH3,MC,MC1,MC2,MC3
100 REAL MOB1,MOB2,MOB3,MOB,MOBH
110 REAL MOBZ
120C
130 DIMENSION CROP(10),PCTG(50),T(10)
140 DIMENSION NN(50),NAI(50),PP(50),NA(50)
150 DIMENSION MD1(10),MD2(10),MD3(10),MD(10)
160C
170 FS(X)=(X-C3)**5*EXP(C3-X)
180 FG(X)=X**15*EXP(-X)
190 F7(X)=(X-C2)**5*EXP(-X)
200C
210 DATA K=4.56,4.27,0.63,4.93/
220 DATA DELTA,M0,K0/0.044,9.10956E-31.438062E-23/
230 DATA HBAR,H*PI/1.05459E-34,6.6262E-34,3.14159/
240 DATA E0,E5/8.854185E-12,11.7/
250 DATA TAU0,WM/6.960E-10,0.244/
260 DATA Q/1.60219E-19/
270 DATA ETA,1,2,3/735.0,0.537,0.153,0.234/
280C
290C READ IN TEMPERATURES AND
300C DENSITY OF STATES EFFECTIVE MASSES
310C READ IN THE H-H SCATTERING CORRECTION
320C FACTOR TO OPTICAL PHONON SCATTERING
330C
340#10 READ(5,10)(T(J),J=1,10)
350#10 READ(5,11)(MD1(L),L=1,10)
360#10 READ(5,11)(MD2(L),L=1,10)
370#10 READ(5,11)(MD3(L),L=1,10)
380#10 READ(5,11)(MD(L),L=1,10)
390#11 FORMAT(10(F7.5,1X))
400#10 READ(5,12)(CROP(L),L=1,10)
410#12 FORMAT(10(F6.4,1X))
420C
430C READ IN DOPANT CONCENTRATIONS
31 MAY 1979

440C READ (5,13)(NA(L),L=1,40)
460C FORMAT(5(E8.2,1X))
470C COMPUTE GAMMA'S AND ASSOCIATED CONSTANTS
490C FOR THE DETERMINATION OF EFFECTIVE MASSES
500C
510 BP=SORT(B**2.+(C**2./6.0))
520 APB=A+BP
530 AMB=A-BP
540 GM=C**2./((2.*BP*AMB)
550 GP=(C**2.1(2.*BP*APB))**(-1.)
560 FM=1.+0.01667*GM+.041359*GM**2.+.00090679*GM**3.+
570 1.00091959*GM**4.0+0.0002106*GM**5.
580 TP=1.+0.01667*GP+.041359*GP**2.+.00090679*GP**3.+
590 1.00091959*GP**4.+.0002106*GP**5.
600 FM=1.+0.01667*GM+.017956*GM**2.+
610 G3P=1.+0.01667*GP+.017956*GP**2.
620 E=0.0069857*GP**3.+0.012510*GP**4.
630C COMPUTE SCATTERING LIFETIME CONSTANTS
640C
650 TOP11=WM*THETA/TAU0
660 TOP22=TOP11
670 TOP33=TOP11
680 TIA=0**2.1SORT(MO)
690 TIB=0**2.1.4.*PI*ES*EO)**2.
700 Tic=TIA**2/((K0**4.5*50155E-7)
710 GA=7.539822E-5*M0/1**2.
720 GB=((ES*EO*4.0*PI)/H)/(K0**2.0/H)
730 GC=GA*GB
740 TNE=1.136E-19/ES**2.
750 TNF=8.88576E6*HBAR**2.0/(M0**1.5*SORT(K0))
760C THIS LOOP CHANGES THE TEMPERATURE
780C
790 DO 200 J=1,8
800 KT=K*T(J)
810 C2=DELTA/(3.*KT)
820 C3=DELTA/CT
830 C4=THETA/T(J)
840 C5=C3+C4
850 C6=C3-C4
31 MAY 1979

860  R8=(MD1(J)/MD(J))**1.5
870  R9=(MD2(J)/MD(J))**1.5
880  R10=(MD3(J)/MD(J))**1.5*EXP(-C3)
890  E=1.205-2.8E-4*T(J)
900  CGAP=(1.205/2)*0.66667
910  M3=3*CGAP
920  WRITE(6,30)
930  FORMAT(I11,/(8X,*CONDUCTIVITY AND HALL EFFECTIVE
940  MASS, CONDUCTIVITY AND HALL MOBILITY,**/Bx,**AND
950  HALL FACTOR AS FUNCTIONS OF DOPANT CONCENTRATION.
960  & BORON DOPED SILICON**/)
970  #30  WRITE(6,40)(J)
980  FORMAT(140X,*T=*,F4.0/)

990  COMPUTE INTERBAND SCATTERING PARAMETERS
1000  Y1=MD1(J)
1010  Y2=MD2(J)
1020  CALL INTBND(Y1,Y2,C11,C12,C21,C12)
1030  INTRODUCE TEMPERATURE AND MASS PARAMETERS
1040  TO THE CALCULATION OF SCATTERING RELAXATION TIMES
1050  AC11=(C11/TAUO)*MD1(J)**1.5*T(J)**1.5
1060  AC22=(C22/TAUO)*MD2(J)**1.5*T(J)**1.5
1070  AC12=(C12/TAUO)*MD1(J)**1.5*T(J)**1.5*
1080  & (MD2(J)/MD1(J))**2.5
1090  AC21=(C21/TAUO)*MD2(J)**1.5*T(J)**1.5
1100  TAC33=1.0/TAU0
1110  AC33=TA33*T(J)**1.5
1120  PDIIST=PDIST**1.
1130  TAC3T=TAC33*T(J)**1.5
1140  PDIST=EXP(C4)**-1.0
1150  OP11=TOP11**SQR(T(J))**MD1(J)**1.5
1160  OP22=TOP22**SQR(T(J))**MD2(J)**1.5
1170  OP33=TOP33**SQR(T(J))**MD3(J)**1.5
1180  T111=T111+(T(J)**1.5*MD1(J)**1.5)
1190  T122=T122+(T(J)**1.5*MD2(J)**1.5)
1200  T133=T133+(T(J)**1.5*MD3(J)**1.5)
1210  T222=T222+(T(J)**1.5*MD2(J)**1.5)
1220  T333=T333+(T(J)**1.5*MD3(J)**1.5)
1230  TNH=TNF/(SQR(T(J))**MD1(J)**1.5)
1240  TNH2=TNF/(SQR(T(J))**MD2(J)**1.5)
1250  TNH3=TNF/(SQR(T(J))**MD3(J)**1.5)
31 MAY 1979

1290C COMPUTE SCATTERING LIFETIMES
1300C THIS LOOP ALSO CHANGES THE CONCENTRATION
1320C DO 100 L=1,40,2
1340C CALL SUBROUTINE TO CALCULATE IONIZED DOPANT DENSITIES
1360C
1370 01=T(J)
1380 02=NA(L)
1390 03=M0(J)
1400 CALL DENSITY(01,02,03,04,05,06,07,08)
1410 NAI(L)=04
1420 PP(L)=05
1430 NN(L)=06
1440 CCTG(L)=07
1450 ETA=08
1460C COMPUTE CORRECTION FACTORS FOR HOLE-HOLE SCATTERING
1480C
1490 IF(NA(L) *LT. 1.0E15) GO TO 44
1500 IF(NA(L) *LT. 3.0E17) GO TO 46
1510 CRAC=0.08
1520 GO TO 48
1530#44 CRAC=1.0
1540 GO TO 48
1560#48 CRAC=1.0004-(A.013378E-19*NA(L))
1560#48 CRI=(NAI(L)/PP(L))*(1.-EXP(-PP(L)/NAI(L)))
1570C INTRODUCE CONCENTRATIONS AND H-H SCATTERING
1580C CORRECTIONS INTO RELAXATION TIME CALCULATIONS
1600C
1610 AC11S=AC11T/CRAC
1620 AC22S=AC22T/CRAC
1630 AC12S=AC12T/CRAC
1640 AC21S=AC21T/CRAC
1660 OP11S=OP11T/CROP(J)
1670 OP22S=OP22T/CROP(J)
1690 OP33S=OP33T/CROP(J)
1690 G1=BT/PP(L)
1700 G2=BT/PP(L)
1710 G3=BT/PP(L)
1720 GB1=ALOG(G1+1.0)-G1/(G1+1.0)
1730 GB2=ALOG(G2+1.0)-G2/(G2+1.0)
```plaintext
1740  GB3=ALOG(G3+1.)-G3/(G3+1.)
1750  TI11=S=TI11T*NAI(L)*GB1/CRI
1760  TI22S =TI22T *NAI(L)*GB2/CRI
1770  TI33S=TI33T*NAI(L)*GB3/CRI
1780  TNI1=TNH1*NN(L)
1790  TNI2=TNH2*NN(L)
1800  TNI3=TNH3*NN(L)
1810C COMPUTE AVERAGE RELAXATION TIMES BY SIMPSON'S RULE
1820C INTEGRATION. FOR BAND 2, 100 ITERATIONS TO GET TO
1830C THE "KNEE" OF THE BAND, AND 200 TO CONTINUE BEYOND
1840C THE "KNEE."
1850C
1860  LIM1=0.02/(K*T(J))
1870  END=50
1880  N1=100
1890  N2=200
1900  N3=300
1910  W=LIM1/(2*N1)
1920  Z=(END-LIM1)/(2*N2)
1930  SUM1=0.0
1940  SUM2=0.0
1950  SUM3=0.0
1960  SUM4=0.0
1970  SUM5=0.0
1980  SUM6=0.0
1990  SUM8=0.0
2000  SUM9=0.0
2010  SUM10=0.0
2020  SUM11=0.0
2030  SUM12=0.0
2040  SUM13=0.0
2050  SUM19=0.0
2060  SUM20=0.0
2070  SUM23=0.0
2080  TLA33 =0.0
2090  X3=0.0
2100  X4=0.0
2110  X5=0.0
2120  X6=0.0
2130  T133=0.0
2140  V=0.0
2150C SET UP SIMPSON'S RULE INCREMENTS
2170C
```
DO 70   KK=1,N3
2190  IF(KK *GT* N1) GO TO 101
2200  GO TO 102
2210 #101  XL=V*2.*(KK-N1-1)*Z
2220  XR=V*2.*(KK-N1)*Z
2230  XM=(XL+XR)/2.*
2240  W=Z
2250  GO TO 103
2260 #102  XL=2.*(KK-1)*W
2270  XR=2.*(KK-1)*W
2280  XM=(XL+XR)/2.*
2290  IF(KK *EQ* N1) V=XR
2300 #103  IF(XL *EQ* 0) XL=XM/1000.*0
2310  DO 65 JJ=1,3
2320  IF (JJ *EQ* 1) X=XL
2330  IF (JJ *EQ* 2) X=XR
2340  IF (JJ *EQ* 3) X=XM
2350 C ACOUSTIC PHONON SCATTERING RELAXATION TIMES
2360 C
2370 C
2380  X1 =SORT(X)
2390  TLAI1 =AC11S*X1
2400  TLAI2 =AC12S*X1
2410  TLAI2 =AC12S*X1
2420  TLAI1 =AC11S*X1
2430  TA33 =AC33S*X1
2440  IF(XL *LT* C3) GO TO 54
2450  TL33 =OP33S*(PDISTI*X3 +PDISTR*X4)
2460  TL33 =OP33S*(PDISTI*X3 +PDISTR*X4)
2470 C CONTINUE
2480 C OPTICAL PHONON SCATTERING RELAXATION TIMES
2490 C
2500  IF(XL *LT* C4) GO TO 57
2510 #57  X6 =SORT(X+C4)
2520 #57  X6 =SORT(X+C4)
2530  TLO11 =OP11S*(PDIST1*X3 +PDIST*X4)
2540  TLO33 =OP33S*(PDIST1*X3 +PDISTR*X4)
2550  IF (XL *LT* C5) GO TO 58
2560 #58  X5 =SORT(X-C5)
2570 #58  IF(XL *LT* C6) GO TO 59
2580  X6 =SORT(X-C5)
2590 #59  TLO33 =OP33S*(PDIST1*X5 +PDISTR*X6)
2600 #59  TLO22 =OP22S*(PDIST1*X3 +PDISTR*X4)
2610 C IONIZED IMPURITY SCATTERING RELAXATION TIMES
31 MAY 1979

2630C  X8 =1.0/X **1.5
2640  T111 =T11S*X8
2650  T133P =T133S*X8
2650  T133P =T133S*X8
2670  IF(XL LT C3) GO TO 63
2680  T133 =T133S/(X-C3)**1.5
2690#63  T122 =T12S*X8
2700C
2710C  NEUTRAL IMPURITY SCATTERING RELAXATION TIME
2720C
2730  X9=X1+TN2/X1
2740  TN1=TN1/X9
2750  TN2=TN2/X9
2760  TN3=TN3/X9
2770C
2780C  TOTAL RELAXATION TIMES IN EACH BAND
2790C  INTRABAND SCATTERING TIMES
2800C
2810  T1 =1.0/ (TLA11 +TL011 +TI11 +TN1)
2820  T2 =1.0/ (TLA22 +TL022 +TI22 +TN2)
2830  T3 =1.0/ (TA33 +TL33 +TI33 +TN3)
2840  TAU3 =1.0/ (TLA33 +TL033 +TI33 +TN3)
2850C
2860  D =1.0-T1 *T2/ (TLA12 *TLA21)
2870  CR1 =1.0+(T2 *MD1(J))/ (TLA12 *MD1(J))
2880  CR2 =1.0+(T1 *MD2(J))/ (TLA21 *MD1(J))
2890  TAU1 =CR1 *T1 /D
2900  TAU2 =CR2 *T2 /D
2910  T3L =1.0/ (R8/TAU1+R9/TAU2+R10/TAU3)
2920  GO TO (1,2,3),J, J
2930#1  TAU1L=TAU1
2940  TAU2L=TAU2
2950  T3L=T3
2960  TAU3L=TAU3
2970  T2L=T2
2980  GO TO 4
2990#2  TAU1R=TAU1
3000  TAU2R=TAU2
3010  T3R=T3
3020  TAU3R=TAU3
3030  T2R=T2
3040  GO TO 4
3050#3  TAU1M=TAU1
3060  TAU2M=TAU2
3070  T3M=T3
31 MAY 1979

TOTAL LIFETIMES IN EACH BAND Squared

TISOL = TAU1L**2.0
TISOM = TAU1M**2.0
TISOR = TAU1R**2.0
T2SOL = TAU2L**2.0
T2SOM = TAU2M**2.0
T2SOR = TAU2R**2.0
T33SOL = TAU3L**2.0
T33SOM = TAU3M**2.0
T33SOR = TAU3R**2.0
T3SQL = TAU3L**2.0
T3SQM = TAU3M**2.0
T3SOP = TAU3R**2.0
TSOL = T3L**2.0
TSOM = T3M**2.0
TSOR = T3R**2.0

SUMMATIONS FOR THE INTEGRALS

SUM1 = SUM1 + (W/3.)*(T3L*F6(XL) + T3M*F6(XM) + T3R*F6(XR))
SUM3 = SUM3 + (W/3.)*(TAU2L*F6(XL) + TAU2M*F6(XM) + TAU2R*F6(XR))
SUM6 = SUM6 + (W/3.)*(T3L*F6(XL) + T3M*F6(XM) + T3R*F6(XR))
SUM8 = SUM8 + (W/3.)*(T33L*F6(XL) + T33M*F6(XM) + T33R*F6(XR))
SUM10 = SUM10 + (W/3.)*(T3L*F6(XL) + T3M*F6(XM) + T3R*F6(XR))
SUM13 = SUM13 + (W/3.)*(TISOL*F6(XL) + TISOM*F6(XM) + TISOR*F6(XR))
SUM19 = SUM19 + (W/3.)*(TSOL*F6(XL) + TSOM*F6(XM) + TSOR*F6(XR))
SUM20 = SUM20 + (W/3.)*(T3SQL*F6(XL) + T3SQM*F6(XM) + T3SQR*F6(XR))
SUM2 = SUM2 + (W/3.)*(TAU3L*F5(XL) + TAU3M*F5(XM) + TAU3R*F5(XR))
SUM9 = SUM9 + (W/3.)*(T3SQL*F5(XL) + T3SQM*F5(XM) + T3SQR*F5(XR))

IF (XL < LT C3) GO TO 66
31 MAY 1979

3435 \( 64 \cdot T3QM \cdot F5(XM) + T3QR \cdot F5(XR) \)
3440 \( SM23 = SUM23 \cdot (W/3.) \cdot (F5(XL) + 4. \cdot F5(XM) + F5(XR)) \)
3450 \#66 CONTINUE
3460 IF(KK GT. NIGO) GO TO 67
3470 SUM4 = SUM4 + (W/3.) \cdot (T2Q2L \cdot F6(XL) +
3475 64 \cdot TAU2M \cdot F6(XM) + TAU2R \cdot F6(XR))
3480 SUM11 = SUM11 + (W/3.) \cdot (T2Q2L \cdot F6(XL) +
3485 64 \cdot T2QM \cdot F6(XM) + T2QR \cdot F6(XR))
3490 GO TO 68
3500 \#67 CONTINUE
3510 SUM5 = SUM5 + (W/3.) \cdot (T2Q2L \cdot F7(XL) +
3515 64 \cdot TAU2M \cdot F7(XM) + TAU2R \cdot F7(XR))
3520 SUM12 = SUM12 + (W/3.) \cdot (T2Q2L \cdot F7(XL) +
3525 64 \cdot T2QM \cdot F7(XM) + T2QR \cdot F7(XR))
3530 \#68 CONTINUE
3540 \#70 CONTINUE
3550C AVERAGE LIFETIMES
3560C
3570C
3580 SUM21 = 1.32934
3590 TAV1 = SUM6/SUM21
3600 TAV2 = SUM3/SUM21
3610 TAV3 = SUM2/SUM23
3620 TAVZ = SUM19/SUM21
3630 TSOV1 = SUM13/SUM21
3640 TSOV2 = SUM10/SUM21
3650 TSOV3 = SUM9/SUM23
3660 TSOVZ = SUM20/SUM21
3670 TRAT1 = TSOV1/TAV1**2.0
3680 TRAT2 = TSOV2/TAV2**2.0
3690 TRAT3 = TSOV3/TAV3**2.0
3700 TRATZ = TSOVZ/TAVZ**2.0
3710C THE INTEGRALS HAVE BEEN CALCULATED
3720C NOW COMPUTE THE MASS
3730C
3740C
3750 R2 = SUM1/SUM2
3760 R3 = SUM3/((F2P \cdot SUM4/\sqrt{AMB}) +
3765 6 \cdot F2M \cdot SUM5/\sqrt{AMB}))
3770 R5 = MD1(J)**1.5/\{\{\sqrt{AMB} \cdot F3W} \}
3780 R6 = MD3(J)**1.5/\{\sqrt{AMB} \cdot \exp(C3)/(\{\{\sqrt{AMB} \cdot SUM9} \)
3790 R7 = SUM10/(F3P \cdot \{\sqrt{AMB} \cdot SUM11} 
3795 \cdot F3M \cdot \sqrt{AMB}) \cdot SUM12)
3800 WCl = MD1(J)**1.5/\{\sqrt{AMB} \cdot F2M}
3810 MC2 = MD2(J)**1.5/\{\sqrt{AMB} \}
31 MAY 1979

MC3=MD3(J)**1.5*SORT(A)*EXP(C3)*R2
MH1=SORT(R5)
MH2=SORT(MD2(J)**1.5*R7)
MH3=SORT(R6)


R11=TAIV1/(TAV2*MC1)
R12=TAIV2/(TAV2*MC2)
R13=TAIV3/(TAV2*MC3)
R14=TSOV1/(TSOVZ*MH1**2*0)
R15=TSOV2/(TSOVZ*MH2**2*0)
R16=TSOV3/(TSOVZ*MH3**2*0)
MC =1./(R11*R8)+(R12*R9)+(R13*R10)
MH =1./SORT(R8*R14)+(R9*R15)+(R10*R16)
MOBI=1.0E4*TAIV1*Q/(MC1*MO)
MOB2=1.0E4*TAIV2*Q/(MC2*MO)
MOB3=1.0E4*TAIV3*Q/(MC3*MO)
MOBZ=1.0E4*TAIVZ*Q/(MC*MO)
RES=1.0/(Q*MOB*NAI(L))
RHZ=TRATZ*(MC/MH)**2
MOB=MOB1+P9*MOB2+R10*MOB3

WRITE OUT COMPUTED VALUES OF MOBILITY, MASS RESISTIVITY, ETC.

WRITE (6,85) NA(L), NAI(L), PP(L), NN(L), PCTG(L)
FORMAT (5X,*NA=*,E10.4,3X,*PP=*,E10.4,3X,*NN=*,E10.4,3X,*NAI/NA=*,F6.4/)
WRITE (6,92) MC1,MC2,MC3,MC
FORMAT (5X,*MC1=*,F7.4,5X,*MC2=*,F7.4,5X)
WRITE (6,96) MH1,MH2,MH3,MH
FORMAT (5X,*MH1=*,F7.4,5X,*MH2=*,F7.4,5X)
WRITE (6,94) MC1,MC2,MC3,MC
FORMAT (5X,*MC=*,F7.4,5X)
WRITE (6,92) MC1,MC2,MC3,MC
FORMAT (5X,MC1=*,F7.4,5X,*MC2=*,F7.4,5X)
WRITE (6,94) MC1,MC2,MC3,MC
FORMAT (5X,*MC=*,F7.4,5X)
WRITE (6,96) MH1,MH2,MH3,MH
FORMAT (5X,*MH1=*,F7.4,5X,*MH2=*,F7.4,5X)
WRITE (6,94) MC1,MC2,MC3,MC
FORMAT (5X,*MC=*,F7.4,5X)
WRITE (6,88) TAIV1,TAIV2,TAIV3,TAIV
FORMAT (5X,*TAIV1=*,E10.4,5X,*TAIV2=*,E10.4,5X)
WRITE (6,89) TSQV1,TSQV2,TSQV3,TSQV
FORMAT (5X,TSQV1=*,E10.4,5X,*TSQV2=*,E10.4,5X)
WRITE (6,88) TAIV1,TAIV2,TAIV3,TAIV
FORMAT (5X,*TAIV1=*,E10.4,5X,*TAIV2=*,E10.4,5X)
WRITE (6,89) TSQV1,TSQV2,TSQV3,TSQV
FORMAT (5X,TSQV1=*,E10.4,5X,*TSQV2=*,E10.4,5X)
31 MAY 1979

4450 WRITE(6,93) TRAT1, TRAT2, TRAT3, TRATZ
4460#93 FORMAT(5X, 'TRAT1=' ,F6.3, 5X, 'T9T2=' ,F6.3, 5X,
4470 'TRAT3=' ,F6.3, 5X, 'TRATZ=' ,F6.3)
4510 WRITE(6,86) C11, C22, C12, C21
4530 1F6.3, 5X, 'C21=' ,F6.3/
4540 WRITE(6,98) M0B1, M0B2, M0B3, M0BZ
4550#98 FORMAT(5X, 'MOB1=' ,F8.2, 5X, 'MOB2=' ,F8.2, 5X,
4560 'MOB3=' ,F8.2, 5X, 'MOBZ=' ,F8.2)
4590 WRITE(6,99) MCB, M0BH, RHZ, RES
4600#99 FORMAT(5X, 'MCB=' ,F8.2, 5X, 'MOBH=' ,F8.2, 5X,
4610 'RHZ=' ,F8.2, 5X, 'RES=' ,F8.2, 5X)
4620C
4630C
4640#100 CONTINUE
4650#200 CONTINUE
4660 WRITE(6,300)
4670#300 FORMAT(1H1)
4680 STOP
4690 END
SUBROUTINE DENSTY (O1, O2, O3, O4, O5, O6, O7, O8)

SUBROUTINE TO CALCULATE IONIZED AND NEUTRAL IMPURITY DENSITY

NV = EFFECTIVE DENSITY OF BAND STATES
EA = DOPANT IONIZATION ENERGY
NA = DOPANT IMPURITY CONCENTRATION
EG = ENERGY GAP
EF = FERMI ENERGY

REAL NV, NA, K, KT, MD
REAL NA, NN
DATA K/8.6173E-5/
DATA DELTA/0.044/
T=0.1
NA=0.2
MD=0.3

CALCULATE EG, NV, AND EA DIVIDED BY KT

EG=(((-3.80977E-13*T +2.95402E-10)*T
--6.701100E-7)*T +.000323741)*T +1.155556

KT=K*T

EAP=(0.0438-3.037E-8*NA**0.3333)/KT

NV=4.82907E15*MD**3.5*T**0.5

ADD=0.0

ITERATION TO FIND A VALUE FOR EF SO THAT P=NA-
IT FINDS EF FOR (P-NA-)< 0.0001

EF=0.43
CD 12 IDEA=L=1,1000
ETA=(EF-EG)/KT
P=NV*EXP(ETA)
IF(ETA .GE. 1.) P=NV*75225*((ETA**2+1.7)**.75)
NAI=NA/(1.*(4.+2.*EXP(-DELTA/KT)))*EXP(ETA)
ADD=EAP
IF(ADD .LE. DIF) GO TO 14

TEST=ABS(P-NAI)
DIF=P/2.
IF(TEST .LE. DIF) GO TO 14

EF=EF+.001
CONTINUE
WRITE(6,13)
FORMAT(/5X*owe fell through loop 0*/)

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5130\#14 \> \( EF = EF - 0.001 + 0.0005 \)
5140 \> DO 15 LI = 1,400
5150 \> ETA = (EF - EG) / KT
5160 \> P = NV * EXP(ETA)
5170 \> IF(ETA .GE. 1.) P = NV * 0.75225 * ((ETA + 2.7) ** .75)
5180 \> NAI = NA / (1. + (4. + 2. ** EXP(-DELTA / KT)) * EXP(ETA))
5185 \& (EAP) \+ ADD
5190 \> TEST = ABS(P - NAI)
5200 \> DIF = P / 100.
5210 \> IF(TEST .LE. DIF) GO TO 30
5220 \> EF = EF + 0.0001
5230\#15 CONTINUE
5240 \> WRITE(6,20)
5250\#20 FORMAT(//5X,* WE FELL THROUGH LOOP 1*/)
5260\#30 EF = EF - 0.001 + 0.0001
5270 \> DO 40 LI = 1,400
5280 \> ETA = (EF - EG) / KT
5290 \> P = NV * EXP(ETA)
5300 \> IF(ETA .GE. 1.) P = NV * 0.75225 * ((ETA + 2.7) ** .75)
5310 \> NAI = NA / (1. + (4. + 2. ** EXP(-DELTA / KT)) * EXP(ETA))
5315 \& (EAP) \+ ADD
5320 \> TEST = ABS(P - NAI)
5330 \> DIF = P / 100.
5340 \> IF(TEST .LE. DIF) GO TO 60
5350 \> EF = EF + 0.0001
5360\#40 CONTINUE
5370 \> WRITE(6,50)
5380\#50 FORMAT(//5X,* WE FELL THROUGH LOOP 2*/)
5390\#60 EF = EF - 0.0001 + 0.00001
5400 \> DO 70 LI = 1,500
5410 \> ETA = (EF - EG) / KT
5420 \> P = NV * EXP(ETA)
5430 \> IF(ETA .GE. 1.) P = NV * 0.75225 * ((ETA + 2.7) ** .75)
5440 \> NAI = NA / (1. + (4. + 2. ** EXP(-DELTA / KT)) * EXP(ETA))
5445 \& (EAP) \+ ADD
5450 \> TEST = ABS(P - NAI)
5460 \> DIF = P / 1000.
5470 \> IF(TEST .LE. DIF) GO TO 90
5480 \> EF = EF + 0.00001
5490\#70 CONTINUE
5500 \> WRITE(6,80)
5510\#80 FORMAT(//5X,* WE FELL THROUGH LOOP 3*/)
5520\#90 ETA = (EF - EG) / KT
5530C \> PP = NAI + NAI * (1. - NAI / NA)
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5550    NN=ABS(NA-NAI+ADD)
5560    PION=(NAI-ADD)/NA
5570    Q4=NAI
5580    Q5=PP
5590    Q6=NN
5600    Q7=PION
5610    Q8=ETA
5620C
5630    RETURN
5640    END
SUBROUTINE INTBND (Y1,Y2,C11,C22,C12,C21,C12)
SUBROUTINE TO CALCULATE INTERBAND RELAXATION TIME
PARAMETERS FOR ACOUSTICAL PHONON SCATTERING.
BOTH LONGITUDINAL AND TRANSVERSE VIBRATIONS ARE CONSIDERED
REAL L211,L111,L222,L122,L212

ETA=0.2125
ETAM=-ETA
ETAMS=ETAM**2
G1=SORT(Y2/Y1)
G2=G1**2
G3=G1**3
G4=G1**4
A=ALOG((1.+G1)/(1.-G1))
BP=(1.+G2)
BPS=(1.+G2)**2

L211=1.-ETAS-2.*ETAM*(1.-ETAM)*P1
L111=(1.+ETA)**2 +3.*ETAS/4.
L222=(1.+ETAM)**2 +3.*ETAM/4.
L122=-ETAMS-2.*ETAM*(1.-ETAM)*P1
L212=(-eta**2+eta**2+15.*etam**4)/(4.*etam**4)
L111t=0.75
L222=0.75
L122=-9.*P5/16.

T111=0.75
T222=0.75
T211=T122
T212=-9.*P5/16.

5650C 5710 5660C 5670C 5680C 5690C 5695C 5700C 5720 5730C 5740 5750 5760 5770 5780 5790 5800 5810 5820 5830 5840 5850 5860C 5870 5880 5884 5890 5891 5892 5893 5894 5895 5900 5905 5910 5915 5920 5925 5930C 5940 5945 5950 5960 5970 5980 5990 5995 6000C 6010 6015 6020 6030 6040 6050
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6060C  C11=L222+G3*L122+2.09*ETAS*(T222+G3*T122)
6070   C22=L211+G3*L111+2.09*ETAS*(T211
6080   +G3*T111)*(Y1**1.5/Y2**1.5)
6090   C12=L212+2.09*ETAS*T212*(Y1**1.5/Y2**1.5)
6100   C21=L212+2.09*ETAS*T212
6110C   P7=3.0*G1*P5/(1-G2)**2.
6120   C112=P7
6130   RETURN
6140C   END
REFERENCES

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BIOGRAPHICAL SKETCH

Luis Carlos Linares was born August 1944 in Bogota, Colombia, and became a United States citizen on December 18, 1964. Raised in Miami, Florida, he attended Miami Central High School, and Miami-Dade Junior College. He received the degree of Bachelor of Science in Electrical Engineering in June 1969, and the degree of Master of Science in Electrical Engineering in December 1970, both from the University of Florida. In March 1971 he entered active service with the United States Air Force and worked until May 1975 as a Computer System Analyst for the Strategic Air Command at Offutt AFB, Nebraska. In June 1975 he was selected by the Air Force Institute of Technology to attend the University of Florida and work toward the degree of Doctor of Philosophy. He is presently a captain in the Air Force, working as an Advanced Communications Requirements Officer, stationed at Scott AFB, Illinois.

Luis Carlos Linares is a member of Eta Kappa Nu and the Institute of Electrical and Electronics Engineers. He is married to the former Diane Hermann, and has three sons, Luis Carlos Jr., John Michael, and Christopher Lee.
I certify that I have read this study and that in my opinion it conforms to acceptable standards of scholarly presentation and is fully adequate, in scope and quality, as a dissertation for the degree of Doctor of Philosophy.

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This dissertation was submitted to the Graduate Faculty of the College of Engineering and to the Graduate Council, and was accepted as partial fulfillment of the requirements for the degree of Doctor of Philosophy.

August 1979
Dean, College of Engineering

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