HOT-ELECTRON NOISE IN GALLIUM ARSENIDE/ALUMINUM GALLIUM

ARSENIDE HETEROJUNCTION INTERFACES

By

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A DISSERTATION PRESENTED TO THE GRADUATE SCHOOL OF
THE UNIVERSITY OF FLORIDA
IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE
DEGREE OF DOCTOR OF PHILOSOPHY

UNIVERSITY OF FLORIDA
1987
ACKNOWLEDGMENTS

The author wishes to express his sincere gratitude to Dr. G. Bosman for his research guidance and many helpful discussions and also to Dr. C.M. Van Vliet and Dr. A. van der Ziel for their support and encouragement. The services of Dr. Morkoc at the University of Illinois in supplying the heterostructures for the experiments are greatly appreciated. He also wishes to thank his fellow students in the Noise Research Laboratory for their help and many interesting discussions and Miss Katie Beard for the editing and typing of the manuscript.

Special thanks go to his wife, Susan, and his family, who have supported and encouraged him over the years.
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Abstract of Dissertation Presented to the Graduate School of the University of Florida in Partial Fulfillment of the Requirements for the Degree of Doctor of Philosophy

HOT-ELECTRON NOISE IN GALLIUM ARSENIDE/ALUMINUM GALLIUM ARSENIDE HETEROJUNCTION INTERFACES

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May 1987

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Major Department: Electrical Engineering

In recent years much attention has been paid to the study of semiconductor heterojunction interfaces. An interest in the hot-electron behavior of electron transport parallel to the interface has arisen.

In this dissertation the charge-transport noise in the direction parallel with the GaAs/AlGaAs interface is studied. Monte Carlo calculations of the electron transport properties of bulk GaAs are fitted to recent experimental data of the field-dependent diffusion coefficient. This method provides a better theoretical value of the Γ-L intervalley coupling constant. The effects of GaAs device length on the velocity fluctuation spectrum are investigated using the Monte Carlo technique. In addition, an experimental investigation of the velocity fluctuation spectrum as a function of electric field and length for different AlGaAs/GaAs heterojunctions is completed. Finally, the dc, ac and noise properties of the AlGaAs/GaAs MODFET channel are investigated both experimentally and theoretically using the impedance field method.
CHAPTER I
INTRODUCTION

In recent years much attention has been paid to the study of semiconductor heterojunction interfaces. Due to increased processing capabilities, novel semiconductor heterojunctions of various material compositions can be manufactured. This opens many new possibilities in the development of existing and novel semiconductor devices and their applications.

In order to take full advantage of these new heterojunctions, more information on the charge-transport properties must be attained. In this dissertation the charge-transport noise in the direction parallel with the GaAs/AlGaAs interface is studied. Monte Carlo calculations of the electron transport properties of bulk GaAs are fitted to recent experimental data of the field-dependent diffusion coefficient. This method provides a better theoretical value of the $\Gamma-L$ intervalley coupling constant. The effects of GaAs device length on the velocity fluctuation spectrum are investigated using the Monte Carlo technique. In addition, an experimental investigation of the velocity fluctuation spectrum as a function of electric field and length for different AlGaAs/GaAs heterojunctions is completed. Finally, the dc, ac and noise properties of the AlGaAs/GaAs MODFET channel are investigated both experimentally and analytically using the impedance field method.

In this introductory chapter the band structure of the AlGaAs/GaAs system is reviewed, including energy band lineup and modulation-doping.
techniques. The second section of this chapter outlines some of the
effects of hot electron behavior on charge transport, such as real-
space-charge transfer vs. intervalley transfer, in providing negative
differential mobility. The length of the active device region can have
a significant effect on the charge-transport properties of GaAs in the
hot electron regime, and this effect is discussed.

Noise measurements have been used for many years as a method for
investigating charge transport properties in materials and devices. A
review of both analytical and computational methods of noise modeling is
presented. Device applications of the AlGaAs/GaAs heterojunction, such
as the heterojunction bipolar transistor (HBT) [1] and the modulation-
doped field-effect transistor (MODFET) [2], are discussed.

1.1. Band Structure of AlGaAs/GaAs

The alloy system Al$_x$Ga$_{1-x}$As/GaAs is of great importance in high-
speed electronic devices since it allows the possibility of bandgap
engineering. The lattice constants between the two materials are
closely matched. If properly grown, this small lattice constant
difference results in high-quality interfaces between GaAs and AlGaAs
with an insignificant concentration of interface states.

The most important device parameter of interest in Al$_x$Ga$_{1-x}$As is
the energy bandgap dependence on the alloy composition. The energy gap
as a function of the mole fraction $x$ can be expressed by [3,4]

\[
E_g(x) = 1.424 + 1.247x (0 < x < 0.45) \quad (1.1a)
\]

\[
E_g(x) = 1.900 + 0.125x + 0.143x^2 (0.45 < x < 1.0) \quad (1.1b)
\]

and the units are in eV. For mole fractions less than approximately
0.45, the AlGaAs has a direct bandgap. For larger mole fractions, the
The alloy bandgap is indirect, with the X-valley having the lowest energy. The L-valley lies between the Γ- and X-valleys for mole fractions larger than 0.45.

The sum of the valence- and conduction-band discontinuities must equal the energy bandgap difference between the GaAs and AlGaAs. Originally, it was believed that the conduction-band discontinuity was 0.85 $E_g(x)$ [5]. However, more recent measurements [6] have shown that sixty-five percent of the bandgap difference lies in the conduction band for $x < 0.45$. Then the conduction-band discontinuity follows from

$$\Delta E_c = 0.81x \text{ (eV)} \text{ for } x < 0.45 .$$

From measurements of the valence-band discontinuity as a function of mole fraction, it was determined that the maximum conduction-band discontinuity lies in the vicinity of $x = 0.45$ [7]. A further increase of the mole fraction results in a decrease in the conduction-band discontinuity with a corresponding larger increase in the valence-band discontinuity.

Of special interest in the AlGaAs/GaAs system is the method of modulation doping. In this doping process, the GaAs layer is undoped and the dopant atoms (usually silicon atoms for n-type) are deposited in the AlGaAs layer. In equilibrium the Fermi level must be constant across the interface. Consequently, the electrons from the donors near the interface transfer to the lower energy GaAs conduction band. In this way, the electrons become spacially separated from the parent donor atoms, causing an electric field normal to the interface. The electric field leads to energy band bending in both the AlGaAs and the GaAs in the vicinity of the heterojunction. This band bending forms a quasi-
triangular potential well for the electrons in the GaAs. If the electric field is large enough, the width of the triangular potential well may be smaller than the carrier deBroglie wave length. The momentum vector perpendicular to the interface then becomes quantized. Shown in Figure 1.1 is an example of a heterojunction where the AlGaAs is doped n-type and the GaAs is slightly p-type.

The modulation-doping process was developed to increase the low-field mobility of electrons in the direction parallel to the interface. At room temperature (300K), the dominant scattering mechanism is polar optical phonon scattering. At lower temperatures, however, the dominant scattering mechanism becomes ionized impurity scattering. Because the electrons are spacially separated from the donor atoms, a reduction of ionized impurity scattering is obtained, leading to a higher electron mobility. The inclusion of a thin spacer layer of undoped AlGaAs between the doped AlGaAs and GaAs reduces even further the coulombic interaction between the donor atoms and free carriers [8].

1.2. Hot-Electron Effects

With microelectronic devices approaching submicron dimensions, even moderate applied voltages result in very high electric fields. These large fields cause the average carrier energy to increase significantly beyond the thermal equilibrium value. This increase in energy leads to nonlinear charge transport (i.e., deviations from Ohm's Law), also known as hot-electron transport. To improve the modeling and performance of electron devices, high-field transport properties need a more thorough understanding.

An interesting hot-electron effect is the occurrence of a negative differential mobility regime in bulk GaAs. This phenomenon, commonly
Fig. 1.1. AlGaAs/GaAs heterojunction at equilibrium.
known as the Gunn effect [9], is due to the transfer of electrons from the high-mobility central Γ-valley to the low-mobility satellite L and X valleys. At low fields the electron velocity increases in proportion to the electric field. At higher field strengths, the electrons partially occupy the low-mobility satellite valleys, and the average velocity is lowered. This net decrease in velocity with increasing field gives rise to the negative differential mobility in GaAs.

From the measurements by Ruch and Kino [10] on bulk GaAs, it was found that the diffusion coefficient shows a sharp increase in the same field range as the onset of transfer of electrons to the satellite valleys. Since the diffusion coefficient is closely related to the velocity fluctuations caused by random scattering, information about the scattering process can be obtained. The increase in diffusion is very sensitive to the intervalley coupling constant $D_{\Gamma L}$. Thus, accurate measurements of the field dependence of the diffusion coefficient can provide a more accurate value for this constant.

Since the L valley is located .33 eV above the conduction-band minimum, it takes time for most electrons to gain sufficient energy under an applied field to undergo intervalley transfer. If the device length is short, few electrons will transfer to the satellite valleys before being collected by the contact. The large changes in velocity associated with intervalley transfer will not occur and less noise will be produced in the external circuit. A description of a Monte Carlo experiment to observe this effect is outlined in Chapter II.

In the AlGaAs/GaAs interface there are two mechanisms that can produce negative differential mobility at high electric fields. The first is the Gunn effect just outlined for bulk GaAs. The second
mechanism is called real-space-charge transfer, which stands for the following physical process. Electrons in the high-mobility GaAs gain energy as they drift under an applied electric field parallel to the interface. When the energy becomes comparable to the conduction-band difference, there is the possibility of transferring to the AlGaAs. Because of the high doping concentration, which introduces a significant amount of ionized impurity scattering in the AlGaAs layer, the electron mobility in this layer is lower than in the GaAs layer. The increasing percentage of electrons transferring to the AlGaAs layer with increasing field causes the drift velocity to decrease, similar to the Gunn effect. Experimentally, real-space-charge transfer has been shown to be the cause of negative differential device conductance of specially made heterostructures [11]. However, accurate modeling of the processes involved is difficult, and even getting experimental verification of negative conductance is rather involved. The length of the heterostructure may also play a role in the transfer of carriers.

Investigation of the field-dependent diffusion coefficient in conjunction with velocity-field measurements should provide information on the hot-electron behavior of the GaAs/AlGaAs interface system. In Chapter III these measurements will be presented for different interface compositions and compared with bulk GaAs.

1.3. Noise Characterization of Hot-Electron Phenomena

Noise measurements are used to provide information on charge-transport processes in semiconductors. In this section the methods of characterizing hot-electron effects by noise measurements are reviewed.

There are basically three types of noise in semiconductor devices: $1/f$, generation-recombination (g-r) and velocity-fluctuation. At low
frequencies $1/f$ and $g-r$ noise, caused by fluctuations in the sample resistance, can be observed by the passage of a current through the sample. The $1/f$ noise mechanism has been attributed to mobility and number fluctuations. Generation-recombination noise is caused by the interaction of carriers with trapping states in the forbidden energy band. The trapping process gives rise to fluctuations in the number of free carriers available for conduction. Velocity fluctuations are a result of carrier interactions with the scattering mechanisms associated with the thermal vibrations of the host crystal. Since the mean intercollision time of the carriers in high-mobility semiconductors is very small, the velocity-fluctuation spectrum extends to very high frequencies. The emphasis in this dissertation is placed on the hot-electron effects that are associated with the various scattering mechanisms. Therefore, velocity fluctuation noise, also known as thermal or diffusion noise, is used as a tool for probing these effects.

Consider a one-port network biased by an arbitrary dc voltage $V_0$ with a dc current $I_0$ flowing through it. The small-signal Thevenin and Norton equivalent circuits, evaluated around the bias point, are depicted in Figure 1.2. In general, the small-signal impedance $Z(V_0,f)$ and admittance $Y(V_0,f)$ are functions of bias and frequency. The voltage and current noise generators represent the noise mechanisms in the network. The mean square voltage fluctuations $\Delta V^2$ can be expressed in terms of the voltage spectral density $S_{\Delta V}$ by

$$\Delta V^2 = \int_0^\infty S_{\Delta V}(V_0,f)df$$

(1.3)  

where $f$ denotes frequency. A similar relation,

$$\Delta I^2 = \int_0^\infty S_{\Delta I}(V_0,f)df ,$$

(1.4)
Fig. 1.2. Thevenin and Norton small-signal equivalent circuits.
holds for mean square current fluctuations in terms of current noise spectral density.

One can now define the concept of an ac noise temperature \( T_n(V_0, f) \) of the network in analogy with the Nyquist relation in the following way:

\[
S_{\Delta V}(V_0, f) = 4k_BT_n(V_0, f)\text{Re}\{Z(V_0, f)\} \\
S_{\Delta I}(V_0, f) = 4k_BT_n(V_0, f)\text{Re}\{Y(V_0, f)\}
\]

(1.5) \hspace{2cm} (1.6)

where \( k_B \) is Boltzmann's constant and \( \text{Re} \{ \} \) stands for the "real part of." It should be noted that the noise temperature is an electrical parameter of the network and has nothing to do with the electron temperature. By connecting a conjugately matched load to the network, the maximum available power is delivered to the load. This maximum available power has the value

\[
P_{av} = k_BT_n(V_0, f)\Delta f
\]

(1.7)

where \( \Delta f \) is the bandwidth of the measuring system. Therefore, \( T_n \) has physical meaning and can be measured. At high frequencies \( (f > 10 \text{ MHz}) \), measurements of \( T_n \) are preferred because it is much easier to measure power flow than terminal voltages and currents.

The above definitions are valid for every one-port network whether it is linear or nonlinear. The following discussion is restricted to homogeneous semiconductor samples for which a one-dimensional treatment is warranted. The link between diffusion coefficient and velocity fluctuations is outlined. It should be noted that the quantum correction factor for thermal noise is neglected [12].
Let the instantaneous velocity of a carrier $i$ at time $t$ be

$$\dot{v}_i(t) = \dot{v}_d(\dot{E}) + \Delta \dot{v}_i(t)$$

(1.8)

where $\dot{v}_d(\dot{E})$ is the average drift velocity and $\dot{E}$ is the electric field. The term $\Delta \dot{v}_i(t)$ represents the fluctuations in the velocity about $\dot{v}_d(\dot{E})$, with the average $\overline{\Delta \dot{v}_i(t)} = 0$. By definition [12] the diffusion coefficient is related to the spectrum of velocity fluctuations by

$$D(E,f) = \frac{S_{\Delta v}(E,f)}{4} = \frac{1}{2} \int_{-\infty}^{\infty} \overline{\Delta v(t)\Delta v(t+\tau)} e^{-j2\pi f \tau} d\tau .$$

(1.9)

where the term $\overline{\Delta v(t)\Delta v(t+\tau)}$ is the autocorrelation function of the velocity fluctuations. At low frequencies eq. (1.9) reduces to the well-known Einstein formula for diffusion

$$\Delta x^2 = 2Dt$$

(1.10)

for sufficiently long $t$.

Consider a semiconductor sample of length $L$ and cross-sectional area $A$ with ohmic contacts. An electron with velocity $\Delta v_i(t)$ gives rise to a current $\Delta i_1(t)$ in the external circuit such that

$$\Delta i_1(t) = \frac{q\Delta v_i(t)}{L} ,$$

(1.11)

and the corresponding spectrum of current fluctuations is

$$S_{\Delta i_1}(f) = \frac{q^2}{L^2} S_{\Delta v}(f) = 4 \frac{q^2}{L^2} D(f) .$$

(1.12)

If the electron gas in nondegenerate and there are $n_{AL}$ electrons in the
sample, then the total noise current spectral density becomes

$$S_{\Delta I}(f) = nAL S_{\Delta I}(f) = 4q^2 \frac{nA}{L} D(f).$$  (1.13)

Using eq. (1.6), one obtains

$$D(f) = \frac{k_B T(f) L}{q^2 nA} \text{Re}(Y).$$  (1.14)

Recognizing that \( \text{Re}(Y) = \text{Re}(\mu')qnA/L \), one arrives at the generalized Einstein relationship

$$D(E,f) = \frac{k_B T(E,f)}{q} \text{Re}(\mu')$$  (1.15)

where \( \mu' \) is the differential mobility. This equation is valid for all cases in which the field remains uniform throughout the sample. As the electric field approaches zero, the noise temperature becomes equal to the lattice temperature, and the Einstein relation reduces to the familiar form in equilibrium

$$D = \frac{k_B T}{q} \mu_0.$$  (1.16)

If the electron gas is degenerate, as in heavily doped semiconductors or metals, electron-electron interactions cannot be ignored. In this case, electrons cannot be treated as statistically independent particles, and cross-correlation terms must be included in the spectrum. Van Vliet and van der Ziel [13] have extended the relation for current spectral density using statistical mechanics and derived
\[ S_{\Delta I}(f) = 4q^2 \frac{nA}{L} D(f) k_B T \left( \frac{\partial \log n}{\partial E_F} \right)_T. \]  

The expression for diffusion in terms of mobility for degenerate semiconductors then becomes

\[ qD(f) \left( \frac{\partial \log n}{\partial E_F} \right) = \text{Re}(\mu'). \]  

Once the sources of noise in semiconductors have been determined, it is possible to characterize the noise at the terminals of solid-state devices. Three methods are used in hot-electron problems: the Langevin, the impedance field, and the transfer impedance. First, in all three methods the equations describing the device behavior are formulated. Then each variable involved is set equal to \( Q = Q_0 + \Delta Q \exp(j\omega t) \). The zero-order terms give the dc characteristics. The first-order terms give the ac equations.

In the Langevin method [14], the appropriate white noise source is added to each ac equation. Auxiliary variables are then eliminated to get a relationship between the ac current \( \Delta I \) and the ac field \( \Delta E \). Writing the solution of \( \Delta E \) in terms of the other variables and integrating over the device length, one gets the ac voltage across the terminals. By setting the noise sources to zero, the device impedance is obtained. Conversely, when \( \Delta I = 0 \), multiplying by the complex conjugate \( \Delta V^* \) results in the ac voltage noise around the bias point. An extensive review of this method was given by Nicolet et al. [15], in application to single-injection diodes.

The impedance-field method was developed by Shockley et al. [16] to describe diffusion noise in devices. In this method the transfer
function between the position-dependent ac current noise sources and the ac voltage at the terminals is derived. Once the transfer function has been obtained, the impedance and noise characteristics easily follow. A general outline of this method applied to a MODFET is reviewed in Chapter IV.

When the variables used to describe the ac properties of a device are written in terms of current ΔI and electric field ΔE, the most general technique for calculating the impedance and noise properties is the transfer impedance method. Van Vliet et al. [17] developed this method to describe the noise behavior in space-charge limited-current (SCLC) solid-state diodes. It was found that the transfer impedance method is quite general and encompasses the impedance-field technique. Its ability was recently utilized by Tehrani et al. [18] in SCLC silicon carbide devices.

As device dimensions continue to shrink, traditional analytical methods of characterizing solid-state devices become questionable. Transient transport effects and boundary conditions will become increasingly important in device modeling. Computer methods for obtaining device noise characteristics are beginning to emerge. In these methods fewer approximations are made concerning carrier transport phenomena; consequently, these methods are expected to lead to more accurate results. In Chapter II the use of the Monte Carlo method to calculate velocity-fluctuation noise is outlined. The technique is then used in modeling noise behavior of very short GaAs diodes.

1.4. Device Applications of Heterojunctions

In the following, two well-known examples of devices based on AlGaAs/GaAs heterojunction operation are discussed.
There are essentially two main parameters that influence the common-emitter current gain $\beta$ in bipolar transistors; they are the emitter efficiency $\gamma$ and the base transport factor. The base transport factor determines how many carriers injected from the emitter into the base reach the collector before recombination occurs. With the short base regions achievable with present processing capabilities, recombination becomes negligible. Then the emitter efficiency, caused by back injection of carriers from the base to the emitter, dominates the current gain. In homojunction technology, the emitter is heavily doped with a lightly doped base region to decrease the back injection. However, the high resistance of the lightly doped base severely limits the high frequency and noise performance of bipolar devices. Doping the base more heavily would lower the resistance but degrade emitter efficiency.

To circumvent these effects, it was proposed by Kroemer [19] that a heterojunction at the emitter-base junction be used. Using a wide bandgap emitter would allow the base region to be heavily doped, thus lowering the base resistance while maintaining high emitter efficiency. This is the basic premise of the heterojunction bipolar transistor (HBT). Much research is currently being pursued on this interesting device topic. Although the technology is available to make heterojunction bipolar transistors today, the processing of integrated circuits is difficult due to layout and interconnection problems.

Heterojunctions have also improved field-effect transistor technology. The Si-SiO$_2$ interface has been used to make MOSFETs for years. However, the interface is often degraded due to surface roughness and interface states. The AlGaAs/GaAs heterojunction does not have
these problems if properly grown. The modulation-doped field-effect transistor (MODFET), also known as the high electron mobility transistor (HEMT), was developed for high-speed applications. In this case the carrier transport is parallel to the interface.

The MODFET fabrication process begins with a semi-insulating GaAs substrate on which an undoped buffer layer of GaAs is grown. A doped AlGaAs layer is then deposited on top of the buffer layer. After ohmic contacts are defined for the source and drain pads, the AlGaAs layer is etched down to provide a Schottky-type gate. The depletion region of the gate is made to overlap the depleted area in the AlGaAs adjacent to the GaAs/AlGaAs interface. Careful control of the gate to interface spacing determines the threshold voltage of the FET structure. A typical MODFET conduction band diagram showing the overlapping depletion regions is shown in Figure 1.3.

The MODFET has shown excellent gain and noise figure characteristics at high frequencies and will probably exceed conventional MESFET capabilities into the millimeter-wave region. In Chapter IV the dc, ac and noise properties of the MODFET channel are derived and experimentally verified.
Fig. 1.3. MODFET conduction band diagram.
CHAPTER II
MONTE CARLO MODELING OF HOT ELECTRON TRANSPORT

The semiclassical Boltzmann transport equation (BTE) describes the evolution of the distribution function in phase space. Once the distribution function is known, the pertinent transport parameters can be obtained by taking the appropriate moments of this function. Solutions of the integro-differential Boltzmann equation can be difficult to obtain analytically. In seeking solutions in the hot-electron regime, drastic approximations have to be made for analytical results.

Monte Carlo techniques were first devised as a computational tool for calculating difficult integral expressions. The general principles have been applied to the solution of differential equations and many other problems in the applied sciences. In this chapter the method of Monte Carlo simulation of electron transport properties in GaAs is examined. The method is very versatile since steady-state as well as transient phenomena can be simulated in situations near as well as far from equilibrium. A main disadvantage of the method is, however, that it requires large amounts of computer time to obtain sufficient statistical accuracy. Therefore, the Monte Carlo technique is not always the most efficient means of investigating a problem.

First, a description of the physical modeling of transport in semiconductors and an explanation of how the Monte Carlo methods are used to describe stochastic processes will be given. Subsequently, the band structure of GaAs in $k$ space and the electron-phonon scattering
mechanisms are reviewed. The sensitivity of the diffusion-field and velocity-field characteristics on the \( \Gamma - L \) intervalley-scattering coupling constant is examined. The proper \( \Gamma - L \) coupling constant is found from fitting the calculated diffusion-field characteristics to recently measured data on GaAs obtained from noise measurements.

Next, the techniques used to obtain the velocity fluctuation spectrum from a velocity time series are described, and results obtained for GaAs under high-field conditions are presented.

As the device length shortens, it is expected that transport behavior becomes more dependent on the imposed boundary conditions. To study the effects of boundary conditions, the Monte Carlo program was modified in such a way that the active device length and initial electron velocity could be adjusted. The effects of the length and boundary conditions on the calculated velocity fluctuation spectrum are examined and compared with bulk behavior.

2.1. Description of Physical Model

The Monte Carlo method can be applied to many physical systems whose parameters are governed by probability distributions. The ability to map simple pseudo-random distributions, available in most computers, into more complex ones is very powerful. The mapping process begins by equating the areas under the different distribution functions. Solving the equations allows one to obtain the physical variable of interest from the known, computer-generated distribution. In the example given by Boardman [20], \( p(r) \) and \( p(\phi) \) are the respective probability densities, where \( r \) is associated with the pseudo-random computer distribution and \( \phi \) is the physical quantity to be obtained from the mapping. Equating the cumulative distributions
\[ \int_{0}^{\phi} p(\phi')d\phi' = \int_{0}^{r} p(r')dr' \quad (2.1) \]

and using a uniform distribution for \( p(r) = 1 \),

\[ r = \int_{0}^{\phi} p(\phi')d\phi' . \quad (2.2) \]

Evaluating the integral of eq. 2.2, one obtains \( \phi \) in terms of \( r \). In the following Monte Carlo program, this method of obtaining random variables is used to generate free-flight times, choose between scattering mechanisms, and select the final \( k \)-space position after scattering. In addition, the energy of the electrons injected into the active device region is calculated using random numbers.

The program to be described is built upon the Fortran version outlined by Boardman [20]. The original Boardman program only allowed for a central valley and one type of satellite valley in the energy-wavevector dispersion relation \( E(k) \) for electrons in the conduction band. Originally, it was believed that the ordering in energy of the conduction-band valleys was \( \Gamma - X - L \) for GaAs in increasing order of electron energy. For this reason the original version included only the \( \Gamma \) and \( X \) valleys, since the \( L \) valley population in this model could be neglected. More recently, it was discovered that the ordering of the valleys is \( \Gamma - L - X \) [21]. The program was rewritten to include all three valleys in the appropriate order. The values for intervalley-scattering coupling constants and energy offsets between valleys were taken from Pozhela and Reklaitis [22]. Figure 2.1 shows the energy-wavevector relationship for the GaAs conduction band. Each valley is taken to be parabolic.
Fig. 2.1. Energy-wavevector relation for GaAs.
Electron motion is most easily described in \( \vec{k} \) space. In simple semiconductors the electrons are regarded as free particles with an effective mass \( m^* \) of the appropriate valley. The electron energy is then given by

\[
E(\vec{k}) = \frac{\hbar^2 k^2}{2m^*}
\]

(2.3)

where \( \vec{k} \) is the reduced wavevector of the electron.

To simulate electron motion, one first generates a random number based on the scattering rates of the valley occupied by the electron. This number is then used to calculate the flight time between collisions. The wavevector \( \vec{k} \) changes during the collision free-flight time in proportion to the applied electric field. If the electric field is in the \(-z\) direction, only the \( k_z \) component of wavevector increases linearly with time during the free flight as indicated by

\[
k_{z_1}(t) = k_{z_f} + \frac{q|\vec{E}|}{\hbar} t.
\]

(2.4)

The subscript \( i \) refers to the initial state before scattering and \( f \) denotes the final state after the previous scattering event. During the free flight the wavevector component \( k_p \) perpendicular to the \( z \) axis does not change. Upon scattering, however, both the \( k_z \) and \( k_p \) components may change and obtain values determined by the particular scattering mechanism involved. This process is shown pictorially in Fig. 2.2.

Having outlined the band structure and concept of electron motion in GaAs, the electron-phonon scattering mechanisms will be reviewed. The program accounts for the following electron-phonon interactions: acoustic phonon (intravalley), polar optical phonon (intravalley),
Fig. 2.2. Electron motion in \( k \) space.
equivalent intervalley (L → L or X → X), and nonequivalent intervalley (L → X, etc.). Intravalley scattering means that the initial and final states before and after scattering are in the same valley, and intervalley scattering means that the two states are in different valleys. Both types of intervalley scattering are via optical phonons since acoustic and polar optical phonon scattering does not allow for large changes in the wavevector.

For all intravalley scattering processes involving optical phonon fields, the energy state after scattering must satisfy the relation

\[ E(k') = E(k) \pm \hbar \omega \]  \hspace{1cm} (2.5)

where \( \omega \) is the radian frequency of the lattice vibration, the plus sign indicates absorption, and the minus sign emission of an optical phonon. Acoustic phonon scattering, however, is treated as an elastic process and therefore \( E(k') = E(k) \).

The energy of the electron is measured with respect to the minimum of the valley it occupies. Therefore, when a nonequivalent intervalley transition occurs, the energy difference between valleys must be accounted for. When the transition is such that the final state is in a valley with a minimum higher in energy than the initial valley, the energy of the electron becomes

\[ E(k') = E(k) \pm \hbar \omega - \Delta , \]  \hspace{1cm} (2.6)

where \( \Delta \) is the energy difference between the valley minima and \( \hbar \omega \) is the optical phonon energy. If the transition is to a valley with a lower minima, then the energy difference is added to the final energy.
Each process that can scatter an electron at the end of a collision free flight is characterized by a transition rate $S_n(\mathbf{k}, \mathbf{k}')$, which is equal to the probability per unit time that an electron is scattered from the state $\mathbf{k}$ to a state $\mathbf{k}'$. The subscript $n$ denotes a particular scattering process. The scattering rate $\lambda_n(\mathbf{k})$ from state $\mathbf{k}$ to any state $\mathbf{k}'$ due to the $n^{th}$ process is found by integrating over all possible final states $\mathbf{k}'$. Hence

$$\lambda_n(\mathbf{k}) = \int S_n(\mathbf{k}, \mathbf{k}') d\mathbf{k}' .$$

The total scattering rate is then found from a summation over all processes

$$\lambda(\mathbf{k}) = \sum_{n=1}^{N} \lambda_n(\mathbf{k}) .$$

The scattering rates for each process are listed in Table 2.1, where the rates are presented in terms of energy rather than in terms of wavevector. The values of the physical constants used to fit experimental data are listed in Table 2.2.

The scattering rates for the central ($\Gamma$) valley are depicted in Fig. 2.3. Polar optical phonon absorption dominates over acoustic phonon scattering at low energy levels. Once the electron energy exceeds an energy of 0.035 eV, it becomes possible to emit a polar optical phonon. The scattering rates for polar optical phonons become smaller as the electron energy increases due to the coulombic nature of the interaction. The dominance of polar optical phonon scattering in GaAs is responsible for the polar runaway phenomena to be discussed later. When the electron energy approaches the energy of the satellite valleys, intervalley transfer plays a role in the total scattering rates. As seen in Fig. 2.3, polar optical phonons still dominate up to
TABLE 2.1
Scattering Rates

<table>
<thead>
<tr>
<th>Mechanism</th>
<th>Scattering Rates $\lambda(E)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acoustic phonon</td>
<td>$\frac{(2m^*)^{3/2}k_BT D_a^2 E^{1/2}}{4\pi p s^2 \hbar^4}$</td>
</tr>
<tr>
<td>(intravalley)</td>
<td></td>
</tr>
<tr>
<td>Polar optical phonon</td>
<td>$\frac{\chi q^2 m^*^{1/2} \omega_0}{4\pi k_0 (2E)^{1/2}} \log \left</td>
</tr>
<tr>
<td>(intravalley)</td>
<td></td>
</tr>
<tr>
<td>Equivalent intervalley</td>
<td>$\frac{(G-1)m^*^{3/2}}{\sqrt{2} \pi \rho \omega_0 \hbar^3}$ $D_e E^{1/2} Y$</td>
</tr>
<tr>
<td>(satellite - satellite)</td>
<td></td>
</tr>
<tr>
<td>Nonequivalent intervalley</td>
<td>$\frac{Gm^*^{3/2}}{\sqrt{2} \pi \rho \omega_0 \hbar^3}$ $D_{ij} E^{1/2} Y$</td>
</tr>
</tbody>
</table>

$Y = N_0$ absorption
$Y = N_0 + 1$ emission
$N_0 = [\exp(\hbar \omega_0 / k_BT) - 1]^{-1}$

$p = \text{material density}$
$s = \text{sound velocity}$
$N = \text{phonon occupation number}$
$\kappa_0 = \text{permittivity of free space}$
$\varepsilon_\infty, \varepsilon_0 = \text{high frequency, static dielectric constants}$
$D_a = \text{acoustic deformation potential}$
$D_e = \text{equivalent intervalley coupling constant}$
$D_{ij} = \text{nonequivalent intervalley coupling constant}$
$E = \text{energy of initial state}$
$E' = \text{energy of final state}$
$G = \text{parameter associated with the symmetry of the valleys}$
<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Material density (g/cm³)</td>
<td>5.37</td>
<td></td>
</tr>
<tr>
<td>2. Sound velocity (10⁵cm/s)</td>
<td>5.22</td>
<td></td>
</tr>
<tr>
<td>3. High-frequency dielectric constant</td>
<td>10.82</td>
<td></td>
</tr>
<tr>
<td>4. Low-frequency dielectric constant</td>
<td>12.53</td>
<td></td>
</tr>
<tr>
<td>5. Optical phonon frequency (10¹³rad/sec)</td>
<td>5.37</td>
<td></td>
</tr>
<tr>
<td>6. Intervalley phonon frequency (10¹³rad/sec)</td>
<td>4.54</td>
<td></td>
</tr>
<tr>
<td>7. Acoustic deformation potential (eV)</td>
<td>7.0</td>
<td></td>
</tr>
<tr>
<td>8. Intervalley coupling constants (10⁹eV/cm):</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Γ - L</td>
<td>0.325</td>
</tr>
<tr>
<td></td>
<td>Γ - X</td>
<td>1.0</td>
</tr>
<tr>
<td></td>
<td>L - X</td>
<td>0.1</td>
</tr>
<tr>
<td></td>
<td>L - L</td>
<td>0.5</td>
</tr>
<tr>
<td></td>
<td>X - X</td>
<td>1.0</td>
</tr>
<tr>
<td>9. Energy separation between valleys (eV):</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Γ - L</td>
<td>.33</td>
</tr>
<tr>
<td></td>
<td>Γ - X</td>
<td>.52</td>
</tr>
<tr>
<td>10. Effective mass (m*/m₀):</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Γ</td>
<td>.063</td>
</tr>
<tr>
<td></td>
<td>L</td>
<td>.17</td>
</tr>
<tr>
<td></td>
<td>X</td>
<td>.58</td>
</tr>
</tbody>
</table>
Fig. 2.3. Scattering rates for $\Gamma$ valley.
about 0.5 eV. Above 0.5 eV the $\Gamma$- to X-valley transitions dominate. The scattering rates in the L and X valleys are shown in Figs. 2.4 and 2.5, respectively.

As mentioned previously, one must generate collision free-flight times from the scattering rates. If $p(t)$ is the probability per unit time that an electron has a flight, of duration $t$, and subsequently scatters, then the flight time $t$ is found from

$$ t = \int_0^r p(t')dt' $$

(2.9)

where $r$ is the uniformly distributed random number. As shown in Boardman [20], eq. (2.9) can be written as

$$ r = 1 - \exp\left\{-\int_0^t \lambda(k)dt'\right\} $$

(2.10)

The integral cannot be evaluated analytically and thus requires numerical evaluation. This involves a significant amount of computer CPU time for each flight. To circumvent this problem, Boardman et al. [23] developed the concept of virtual scatterings. In a virtual scattering event, the state of the electron does not change. The scattering rate for the electron, including virtual scattering, becomes equal to

$$ \text{GAMMA} = \lambda_T(k) + \lambda_V(k) $$

(2.11)

where GAMMA is the nomenclature used by Boardman, and $\lambda_V$ is the virtual scattering rate. Since GAMMA is a constant, the integral in eq. (2.10) can be easily evaluated, and one finds for $t$

$$ t = -\log(r)/\text{GAMMA} $$

(2.12)

The value of GAMMA is usually taken to be equal to the maximum electron real scattering rate evaluated over the possible electron energy range.
Fig. 2.4. Scattering rates for L valley.
Fig. 2.5. Scattering rates for X valley.
At the end of a collision free flight, the electron is scattered by one of the real processes or by a virtual process. The scattering rate for each process is evaluated and normalized to unity by dividing by GAMMA. A random number is generated uniformly between 0 and 1 to choose between scattering mechanisms. If a virtual scattering mechanism is chosen, the wavevector $\vec{k}$ remains the same and the program proceeds to generate a new flight time. However, if a real scattering mechanism is chosen, a new wavevector must be stochastically determined before a new flight time can be produced. A block diagram of the electron transport simulation is outlined in Appendix A.

At the end of a sufficiently long time interval to obtain convergence, the quantities of interest such as the mean velocity, the diffusion coefficient, etc., are evaluated and outputed. More details can be found in Boardman [20].

2.2. Determination of Γ-L Intervalley Coupling Constant and its Relation to the Diffusion-Field Characteristics

Recently obtained experimental data [24,25] of the field-dependent diffusion coefficient of GaAs at room temperature can be combined with Monte Carlo calculations to investigate transport parameters. Input variables to the program such as effective masses, valley separations in energy, deformation potentials, etc., can be adjusted to give a proper fit to experimental data. The most uncertain of these transport parameters are the intervalley scattering coupling constants, which represent the strength of the electron transfer mechanism resulting in intervalley transitions via a deformation potential. According to recent literature [5], these constants have values that range from $10^8$ to $10^9$ eV/cm for GaAs.
At low electric fields the inter-valley transitions play a minor role in transport since most of the electrons stay in the central (\(\Gamma\)) valley. With larger fields present, the electrons move to higher energies in the conduction band, thus enabling the inter-valley transfer from \(\Gamma\) to \(L\) valleys. This inter-valley transfer to the low-mobility satellite valleys is the cause of the negative differential mobility regime in bulk GaAs.

Shown in Fig. 2.6 is the variation of the velocity-field characteristic as a function of the \(\Gamma-L\) inter-valley coupling constant. The minimum and maximum values of the constant were obtained from other Monte Carlo simulations of bulk GaAs [20,22]. It can be seen that the maximum sensitivity of the velocity-field relationship lies in the 3 to 5 kV/cm range. This is the same range where Gunn oscillations of bulk GaAs make accurate measurements almost impossible.

Figure 2.7 unveils the effect of changing the \(\Gamma-L\) inter-valley coupling constant on the field-dependent, low-frequency diffusion coefficient of GaAs. Measurements, utilizing noise techniques, of the diffusion coefficient of GaAs done by Bareikis et al. [24] and Gasquet et al. [25] are included in the figure. Accurate noise measurements can be done below 3 kV/cm without the problems associated with Gunn domain formation. There is a strong peak in the diffusion coefficient around 3 kV/cm that is very sensitive (much more so than the velocity) to the \(\Gamma-L\) inter-valley coupling strength. The value of \(0.325 \times 10^9 \text{ eV/cm}\) gives the best fit to the experiments.

The increase in the diffusion coefficient with electric field in bulk GaAs has been attributed to two mechanisms, inter-valley transfer
Fig. 2.6. Velocity-field characteristics of bulk GaAs vs. $\Gamma$-L intervalley coupling constant.
Fig. 2.7. Normalized diffusion-field characteristics of bulk GaAs vs. T-L intervalley coupling constant. Measured values indicated by circles and squares are from Bareikis et al. [24] and Gasquet et al. [25], respectively.
and polar runaway. In both of these mechanisms the intervalley coupling strength has an effect on the diffusion coefficient.

Electrons undergoing intervalley transfer experience large changes in velocity due to the randomizing nature of the intervalley process and due to the change in effective mass. These large fluctuations in velocity might be responsible for the increased diffusion coefficient. As can be seen in Fig. 2.8, the population of the L valley starts to increase, due to intervalley transfer, in the same field range where the diffusion coefficient increases.

Polar runaway is a term used to describe a process attributed to semiconductors in which polar optical phonon scattering dominates [26]. Since polar optical phonons emphasize small-angle scattering, the electrons heat up fast. In addition, the process becomes less efficient with increasing electron energy. Consequently, fast electrons move even faster. This causes the velocity distribution to widen, corresponding to an increase in $\Delta v^2$. Assuming that the correlation time of velocity fluctuations is not significantly altered in this process, the low-frequency diffusion coefficient (plateau value) will increase with electric field (see eq. 1.9).

Figure 2.9 shows the results of a Monte Carlo simulation of the frequency dependence of the diffusion spectrum for different electric field strengths. In this simulation all electrons were confined to the central valley as no intervalley transfer was allowed. As Fig. 2.3 indicates, polar optical phonon scattering dominates in this case. The spectral shape remains essentially unaltered while the plateau value increases with field strength. This confirms the fact that the velocity distribution spreads ($\Delta v^2$ increases), while the time dependence of the
Fig. 2.8. Average L and X valley population of bulk GaAs vs. $\Gamma$–L intervalley coupling constant.
Fig. 2.9. Diffusion spectra vs. electric field for electrons in Γ valley (polar runaway).
velocity autocorrelation function experiences little change. Section 2.3 will explain how the calculations of the spectrum are made.

It is expected that when all three valleys are included in the simulation, a decrease of the Γ-L intervalley coupling constant will cause the electrons in the central valley to have a smaller probability of scattering to the L valley. Since the probability of intervalley scattering is smaller, the electrons spend more time, on the average, in the central valley where polar optical phonon scattering dominates. If polar runaway is the cause of increased diffusion, then decreasing the Γ-L intervalley coupling strengths would result in an increase in the diffusion coefficient as indicated in Fig. 2.7. However, when one observes that the decreased coupling constant gives rise to a larger average electron population in the L valleys, the effects of polar runaway are not as clear. As a result of the decreased coupling strength, once the electron scatters to the L valley there is a small probability of returning to the central valley. This is the cause of the average L valley population increase.

2.3. Monte Carlo Spectral Analysis of Velocity Fluctuations

Since the diffusion coefficient is a frequency-dependent parameter as shown by eq. (1.9), it is interesting to investigate the velocity-fluctuation spectrum to gain insight into transport processes. In this section the process of how to generate the velocity time series in the Monte Carlo program is described, including the selection of sampling rate. The definition of spectral density is reviewed, and the calculation of the spectrum from discretely sampled signals is explained. Results for bulk GaAs are presented, and they indicate the effects of a dominant scattering process on the spectrum.
The Nyquist sampling theorem states that the sampling rate \( f_s = 1/\Delta t \) must be at least twice the highest frequency component of the waveform being sampled. Here, \( \Delta t \) is the length of time between samples. If the sampling rate is less than twice the highest frequency present, then aliasing will occur. In other words, the sampling time \( \Delta t \) used in the Monte Carlo program must be much smaller than the intercollision time. After considering the scattering rates in GaAs (see Figs. 2.3 - 2.5), the sampling time of \( 5 \times 10^{-15} \) sec was chosen, reducing aliasing to a negligible effect. However, after observing the spectral characteristics of GaAs, the sampling time was increased to \( 2.5 \times 10^{-14} \) sec to reduce the time-series length.

To obtain the velocity time series, the program first generates the free-flight time of the electron between scattering events, as described in section 2.1. The collision free-flight time is then broken up into smaller subflights of duration \( \Delta t \). The subflights are treated similarly to the virtual scattering process. At the end of each subflight, the velocity of the electron is calculated from the knowledge of the wavevector component \( k_z \) in the direction of the applied field. In principle one could also sample the velocity components normal to the field direction. This would allow characterization of the transverse diffusion coefficients. The velocity of the electron in one dimension is given by

\[
  v_z = \frac{1}{\hbar} \frac{\partial E(k)}{\partial k_z} = \frac{\hbar k_z}{m}. \tag{2.13}
\]

These subflights continue until the end of the free flight or the time window length \( T_s = N \Delta t \) has been reached.
The actual algorithm of the process is described below and outlined in the flow chart of Appendix B. Since scattering events occur, in general, between the sampling times, the computer must keep track of when it last took a sample. The program labels the time passed since the last sample was taken as TIMEX. When the free-flight time between scattering events (TIME) is generated, the algorithm first determines whether the generated time (TIME) plus the time remaining since the last sample (TIMEX) is long enough to reach the next sampling time. If it is not, the flight time is added to TIMEX to become the new TIMEX, and the program proceeds to the next scattering selection without taking a sample of the velocity. When the generated free-flight time plus TIMEX is greater than the sampling time $\Delta t$, the program advances to the next sampling time by the time labeled $\text{TIME}_V = \Delta t - \text{TIMEX}$. The velocity of the electron is then calculated using eq. (2.13) and stored in the time series. Figure 2.10 pictorially represents the relationship of the times in the sampling process.

The number of samples in the time series that can be taken in the remaining free-flight time is designated by $NN$. The value of $NN$ is an integer number and is determined by dividing the remaining flight time by $\Delta t$ and truncating any fractional quantity. When $NN$ is equal to zero, the remaining time is not long enough to reach the next sampling time, so the remaining time becomes TIMEX. The program then goes to the next scattering selection. For $NN$ greater than zero, the algorithm loops through $NN$ subflights, generating additional time-series data. At the end of the $NN$ loop the new value of TIMEX is updated by the remaining time before the loop minus the loop time. The program then proceeds to the next scattering selection.
Fig. 2.10. Representation of times used to generate velocity time series.
The number of samples \( N \) in the time series is monitored at each sampling time. When the number reaches \( T_s/\Delta t \), the program stops sampling and proceeds to the FFT algorithm.

The methods of calculating the velocity-fluctuation spectral density from the time series will now be reviewed. Here we follow the outline given by Tehrani [27]. Let a random signal \( x(t) \) in the interval \( 0 < t < T_s \) be defined in terms of a Fourier series

\[
x(t) = \sum_{K=\infty}^{\infty} a_K e^{j2\pi f_K t}
\]

where \( f_K = \frac{K}{T_s} \) \((K = 0, \pm 1, \pm 2 \ldots)\) and \( a_K \) is the Fourier coefficient of \( x(t) \) at \( f_K \). The discrete Fourier coefficients \( a_K \) are defined as

\[
a_K = \frac{1}{N\Delta t} \sum_{n=0}^{N-1} x(n\Delta t) e^{-j2\pi f_K n\Delta t}
\]

where \( x(n\Delta t) \) is the sampled time data, \( \Delta f \) is the frequency spacing defined as \( \Delta f = 1/N\Delta t \), and \( K \) denotes the frequency component \( f_K = \frac{K}{N\Delta t} = K\Delta f \). The Fourier component \( X_K \) of \( x(t) \), having a frequency \( f_K \), is given by

\[
X_K = a_K e^{j2\pi f_K t} + a_{-K} e^{-j2\pi f_K t}.
\]

The ensemble average of \( X_K^2 \) is found to be

\[
\overline{X_K^2} = 2 a_K a_{-K}
\]

since the Fourier coefficients have an arbitrary phase resulting in
\[ a_K = a_{-K} = 0, \text{ and since for a real signal } x(t) \]

\[ a_{-K} = a_K^* . \] (2.18)

Writing the ensemble average in terms of the discrete Fourier transform results in

\[ \overline{X_K^2} = \frac{2}{N\Delta t} \sum_{n=0}^{N-1} \sum_{m=0}^{N-1} (\Delta t)^2 x(n)x(m) \exp(j2\pi f_K(m-n)\Delta t) . \] (2.19)

For a stationary process and setting \( s = m-n \), the two summations can be decoupled as shown in [27], resulting in

\[ \overline{X_K^2} = \frac{2}{N\Delta t} \sum_{s=-M}^{M} \Delta t \overline{x(n)x(n+s)} \exp(j2\pi f_K s\Delta t) . \] (2.20)

Since \( \overline{x(n)x(n+s)} = 0 \) for \( s>M \) and if \( N>M \), the limits of summation change such that

\[ \overline{X_K^2} = \frac{2}{N\Delta t} \sum_{s=-\infty}^{\infty} \Delta t \overline{x(n)x(n+s)} \exp(j2\pi f_K s\Delta t) . \] (2.21)

The spectral density of \( x(t) \) can be defined by the discretized Wiener-Khintchine theorem,

\[ S_x(f_K) = 2 \sum_{s=-\infty}^{\infty} \Delta t \overline{x(n)x(n+s)} \exp(j2\pi f_K s\Delta t) , \] (2.22)

which is essentially the Fourier transform of the discretized auto-correlation function \( \overline{x(n)x(n+s)} \) of the process \( x(t) \). Since \( \Delta f \) is the frequency interval between adjacent \( f_K \)'s, the spectral density can be written as
Equations (2.22) and (2.23) show that there are two routes that can be taken to calculate the spectral density of a signal. One can either generate the discretized autocorrelation function from the time series and then compute the Fourier transform, or one can calculate the Fourier coefficients \( a_k \) directly by fast Fourier transform (FFT) and average each spectrum. The latter method was preferred in this case since it involves calling only one of the standard library subroutines available on the Harris 800 computer system. Computing the spectrum from the autocorrelation function would require calling two subroutines, one to compute the autocorrelation function and another to take the Fourier transform. This method would be more time consuming.

The Harris subroutine used is named FFTRC. This subroutine computes the fast Fourier transform of a real valued sequence. Time-series lengths up to \( N = 20,000 \) have been transformed by the subroutine very quickly and without any problems. All variables transferred to the subroutine must be defined in single precision. Since many of the variables used in the Monte Carlo program are implemented in double precision for accuracy, the data to be passed on are stored in single-precision variables before calling the subroutine.

The computer program proceeds as follows. First, the program computes the average value of the velocity time series and subtracts it from the data. This new time series is then stored in the single-precision real vector \( \mathbf{A}(G) \). A running average of the average velocity is made for each time series. The vector \( \mathbf{A}(G) \) is the data to be transformed by the FFT. The output is expressed in the complex vector \( \mathbf{X}(G) \).
The FFT algorithm computes the following summation:

\[ X(K) = \sum_{j=0}^{N-1} A \left(-\frac{jT}{N}\right) e^{j2\pi kj/N}. \]  \hspace{1cm} (2.24)

Therefore, the spectral density at frequency \( \frac{K}{T_s} \) of the time series is found by multiplying \( X(K) \) by its complex conjugate \( X^*(K) \), then multiplying the result by \( \frac{2T_s}{N^2} \) and averaging over many time series. The velocity-fluctuation spectral density is then calculated from

\[ S_{AV}(K) = \frac{2T_s}{N^2} \frac{X(K)X^*(K)}{N}. \]  \hspace{1cm} (2.25)

In order to obtain the diffusion coefficient, one simply divides the velocity-fluctuation spectral density by 4, as indicated in eq. (1.9). The average diffusion spectrum is stored in the vector \( AV(\mathbf{G}) \). The constant \( \frac{2T_s}{4N^2} \) is lumped into a single number to improve computation time. Although the first \( N/2 + 1 \) coefficients of the Fourier transform are available, only the first 400 frequencies were outputed for our purposes. The time window \( T_s \) was chosen to be 100 ps, giving a frequency resolution \( \Delta f = 1/T_s \) of 10 GHz.

We are now in a position to calculate the velocity-fluctuation spectral density of bulk GaAs at room temperature (300 K). Calculations of the low-frequency diffusion coefficient \( D(E,0) \) as a function of electric field, using the time-of-flight and spectral-density methods, show good agreement.

At each field strength the spectra have been normalized to their low-frequency plateau level so that the relative spectral shapes can be compared, as shown in Figs. 2.11 and 2.12. For the low-field range,
Fig. 2.11.Normalized diffusion coefficient spectral density for 3 and 5 kV/cm.
Fig. 2.12. Normalized diffusion coefficient spectral density for 7, 10, and 20 kV/cm.
between 1 and 3 kV/cm, the spectrum has a Lorentzian shape with a half-power bandwidth on the order of 500 GHz. At 5 kV/cm a peak shows up in the spectral characteristics around 300 GHz. As indicated in Fig. 2.12, the peak in the spectra moves gradually to higher frequencies as the field increases. The presence of a peak in the spectrum was first observed in Monte Carlo simulations of InP and explained by Hill et al. [28]. The peak has also been observed in simulations of GaAs done by Fauquembergue et al. [29] and Grondin et al. [30].

The observed peak in the spectrum has been attributed [28] to a strong scattering cycle of electrons from a satellite valley back to the central valley with a velocity in the direction negative to the motion under the applied field. The electrons are then accelerated under the applied field through the valley minima and travel almost ballistically until they scatter once again to the satellite valley. This scattering process is pictorially shown in Fig. 2.13. The ballistic motion is characterized by an almost sawtooth-like velocity waveform as indicated in Fig. 2.14, where the associated Fourier spectrum of this waveform is also presented. As the electric field increases, the motion through the central valley becomes faster, causing the peak in the spectrum to move higher in frequency as displayed in Fig. 2.12.

2.4. Position Monitoring and Boundary Conditions in Monte Carlo Programming

It is expected that as device dimensions shrink to submicron levels, the boundary conditions and the length of the active region will have significant effects on the charge-transport characteristics of these devices. To investigate these phenomena, the Monte Carlo program
Fig. 2.13. Scattering process responsible for spectral peak.
Fig. 2.14. Dominant scattering process: a) velocity waveform; b) spectral characteristics.
was rewritten to monitor the electron position in real space. Electrons can be injected from a cathode at some well-defined position \((z = 0)\) and removed at the anode after drifting some fixed length \(L\). The injected electron energy at the cathode can be tailored to any probability distribution desired.

The program still contains the velocity time-series capability so that the velocity spectral density information of short-channel devices is obtained. This method is physically satisfying, in that it is analogous to the measurement of noise in actual devices. The program does not, however, account for noise associated with the injection process. Also, the effects of space charge are neglected by assuming a uniform electric field throughout the active device region.

An outline of the algorithm to monitor the position of the electron in real space is given below. This will include a description of the back scattering of electrons from the active region into the cathode. Although the back-scattered electrons do not contribute to the dc characteristics, they do have an effect on the velocity spectrum. Thus, it is important to include the back scattering in the simulation.

When an electron reaches the anode or returns to the cathode, a new electron is injected. The injected electron velocity is derived from a modified Maxwellian velocity distribution [31].

After explaining how the program functions, results for different-length GaAs devices will be presented. The experimental data of Andrian [32] on 1.1 μm GaAs diodes will then be compared with the simulations.

2.4.1. Program algorithm

The equations describing electron motion, in one direction, during the free-flight time between collisions can be expressed most simply in
terms of a classical velocity
\[ v_z = v_0 + at \] (2.26)

and position
\[ z = z_0 + v_0 t + \frac{1}{2} at^2 \] (2.27)

where \( t \) is time, \( v_0 \) is the initial velocity, \( z_0 \) is the initial position, and the acceleration \( a \) is given by \( q|E|/m^* \). At the beginning of the simulation, an electron is injected with some positive initial velocity, derived from the modified Maxwellian velocity distribution, at the position \( z = 0 \). The Monte Carlo program then generates the collision free-flight time according to the standard procedure as outlined in section 2.1.

The first thing that has to be determined at the beginning of each collision free flight is whether at any time during the flight the electron ever goes back into the cathode. In other words, a check is made to see if the electron position becomes negative \( (z < 0) \). The position of the electron obeys a quadratic equation (2.27) in time and depends on the direction of the initial velocity. If the initial velocity is positive, then the electron position only increases with time. However, when the initial velocity is negative, the position first decreases and then increases given that the flight time is long enough. Therefore, to determine if the electron ever goes back into the cathode, the program only has to check those flights in which the initial velocity is less than zero.

With a negative initial velocity, the program first calculates the time in which the electron velocity \( v_z \) is equal to zero. This time,
labeled $T_{MIN}$, corresponds to the minimum position of the particle during the flight if the flight time is at least that long. The value of $T_{MIN}$ is determined by

$$T_{MIN} = \frac{-v_0}{a}. \quad (2.28)$$

A check is made to determine whether the flight time ($TIME$) is less than $T_{MIN}$. If it is less than $T_{MIN}$, the minimum position is determined by the flight time. The minimum position $Z_{MIN}$, during the electron flight, is now calculated from (2.27) using $T_{MIN}$ or $TIME$, whichever is smaller.

When $Z_{MIN}$ is less than zero ($Z_{MIN} < 0$), the program calculates at what time during the flight $Z_{MIN} = 0$. Solving (2.27) for the time when $z = 0$, one obtains

$$t = \frac{-v_0 - \sqrt{v_0^2 - 2az_0}}{a}, \quad (2.29)$$

since the smaller of the two roots of the quadratic equation corresponds to the first time the electron crosses the boundary. This new calculated time (2.29) is the actual flight time of the electron in the active region. Now the velocity time series can be updated for this flight.

A flag in the program, labeled IFLAG, is set equal to 1 each time that $Z_{MIN}$ is found to be less than zero. This flag causes the program to reinject another electron from the cathode after the time series has been updated. The value of 1 is assigned to the flag to keep track of how many electrons scatter back into the cathode during the simulation. The number of back-scattered electrons is stored in the variable ILTO.
When the initial velocity is positive or the minimum position is found to be still in the active region, the program determines the final position from (2.27), using the free-flight time. This final position is compared to device length L to see if the electron was collected by the anode. When \( z < L \), the time series is updated during the free flight and then proceeds to the next scattering selection. If the final position is greater than L, the exact time that the electron passed the anode boundary must be calculated. This new flight time is

\[
t = \frac{-v_0 + [v_0^2 - 2a(z_0-L)]^{1/2}}{a}
\]

(2.30)

and is used in updating the time series. As before, the flag is set when the electron reaches the anode, indicating injection of another electron from the cathode. This time, though, the flag value is equal to 2 so as not to interfere with keeping track of the number of back scattering. A block diagram of the position-monitoring algorithm is given in Appendix C.

During the process of evaluating the velocity time series, the counter \( N \) is monitored. When the appropriate time window length \( T_s (= N\Delta t) \) is reached, the program proceeds with the spectral density calculations as outlined in section 2.3.

Every time the electron arrives at the anode or scatters back to the cathode, a new, central-valley electron is injected into the active region to maintain constant space charge. The electrons injected in the \( z \) direction obey a modified Maxwellian distribution [31]. The probability that an electron is emitted with a velocity between \( v_z \) and \( v_z + \Delta v_z \) is
\[ \Delta P(v_z) = \exp \left( -\frac{1}{2} \frac{mv_z^2}{k_B T} \right) \Delta \left( \frac{1}{2} \frac{mv_z^2}{k_B T} \right), \quad (2.31) \]

where \( T \) is the lattice temperature. The modified Maxwellian distribution can be generated from a uniform distribution with the techniques of section 2.1. Here the variable \( EZ \), associated with the energy due to the \( v_z \) component, is randomly generated from \( r \), using

\[ EZ = -k_B T \log(r). \quad (2.32) \]

The average value of this distribution is \( k_B T \).

The wavevector (or velocity) component is found directly from \( EZ \) by

\[ k_z = \left( \frac{2m^*EZ}{\hbar^2} \right)^{1/2}. \quad (2.33) \]

Only the positive root need be taken since negative values signify electron motion back into the cathode.

The emitted electrons also have velocity components perpendicular to the field direction. These electrons obey a Maxwellian distribution in each direction. The energy distribution associated with the perpendicular velocity components can be expressed in a form similar to (2.31), so the wavevector component \( k_p \) is determined in much the same way using (2.32) and (2.33). The actual magnitudes of the two perpendicular components \( k_x \) and \( k_y \) are not needed since the program simulation considers the \( x-y \) dimensions to be infinite. However, the two components can be determined by generating a random phase angle between 0 and \( 2\pi \) once the magnitude of the \( k_p \) wavevector is known. This would need to be done to gain information on the transverse diffusion coefficient.
Both perpendicular components have an average energy equal to $\frac{1}{2} k_B T$. Therefore, the total average energy of injected electrons into the active region is $2 k_B T$ [31].

An integer variable named IINJ is used to keep track of how many electrons are injected from the cathode. The difference between IINJ and the number of electrons returning to the cathode ILTO gives the number of electrons traversing the entire length of the active region to the anode. A copy of the entire program is listed in Appendix D.

2.4.2. Simulation results

The program was run for GaAs at room temperature (300 K) with the same intervalley coupling parameters used to fit the bulk experiments in section 2.2. The length of the active region was varied from 0.25 to 4 $\mu$m, and the values at the electric field were chosen between 1 and 3 kV/cm. A number of interesting effects on transport behavior versus device length can be observed in the results presented in Table 2.3.

First, when the electrons are injected into the active region, they are rapidly accelerated by the electric field to very high velocities. If the device length is short, the electron velocity has insufficient time to relax to the steady-state bulk velocity before being collected by the anode. This transient velocity phenomenon is termed velocity overshoot [33]. As shown in Table 2.3, for a given field value as the device length is reduced, the average velocity throughout the active region increases. This increase in average velocity signifies the occurrence of velocity overshoot near the cathode.

Second, the amount of intervalley transfer, from $\Gamma$ to $L$ valleys, is reduced in short devices. In Fig. 2.15 the average fraction of time spent in the $L$ valley during the simulation of 3 kV/cm as a function of
<table>
<thead>
<tr>
<th>Length (µm)</th>
<th>Electric Field (kV/cm)</th>
<th>$\bar{v}$ ($10^7$ cm/s)</th>
<th>$S_{\Delta v}(0)/4$ (cm$^2$/s)</th>
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<tr>
<td></td>
<td>3</td>
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</table>
active region length is presented and compared to the bulk GaAs value. Injected electrons with high energies, near the \( \Gamma - L \) energy offset of 0.33 eV, can undergo intervalley transfer after traveling over short distances. However, since most of the injected electrons have low initial energy \( (E_{av} = 2 k_B T) \), they must travel farther into the active region before gaining sufficient energy for \( \Gamma - L \) intervalley transitions to commence [34]. Therefore, as the length of the active region decreases, a higher fraction of the injected electrons are swept out at the anode before transferring to the \( L \) valley.

The velocity fluctuation spectrum is also determined as a function of device length. Table 2.3 gives the low-frequency plateau value of the spectrum for each length and field. As mentioned before, shot noise behavior associated with the random injection of electrons from the cathode is not taken into account. Often in real device structures the injection noise levels are reduced due to space-charge suppression [35]. Only the effects of the velocity spectrum in the active region are calculated and presented.

The spectrum plateau levels are normalized to the low-field value at each length and depicted in Fig. 2.16. This figure shows the relative increase in the noise characteristics versus field strength for various device lengths, as well as for a bulk device. Also included in the figure are the normalized diffusion coefficient measurements of a \( n^+ - n - n^+ \) GaAs mesa structure, performed by Andrian [32]. The donor concentration in the 1.1 \( \mu m \) active \( n \)-layer was \( 10^{15} \) cm\(^{-3}\). The Monte Carlo data support the measurements, showing that the relative increase in the current-noise spectral density measured in short GaAs regions is not as large as for bulk GaAs.
Fig. 2.15. Fraction of time electrons spent in L valleys at 3 kV/cm as a function of active region length.
Fig. 2.16. Relative increase in GaAs low-frequency velocity spectral density versus electric field for several active region lengths.
Again, the mechanisms causing the increase in the low-frequency velocity spectrum with increasing field can be due to intervalley transfer or polar runaway. In very short active regions, the lower noise produced could be attributed to the decrease in intervalley transfer. It can also be argued that for the short regions there is insufficient scattering before the electrons are removed at the anode, so the spread in the velocity distribution attributed to polar runaway cannot be attained.
In this chapter, we will discuss the experiments which are done to determine the dc, ac and noise properties in the hot-electron regime of AlGaAs/GaAs heterojunction interfaces. Two device structures with different characteristics, such as length, fraction of aluminum content, sheet-carrier concentration, etc., are used in the experiments.

In this dissertation the emphasis is on noise characterization, so first a review of the methods of measuring the device ac noise temperature $T_n$ is given. With the use of noise temperature data, the diffusion coefficient can be determined as a function of electric field for transport parallel to the AlGaAs/GaAs interface. The differences in the experimental results between the two interfaces are examined and compared to bulk GaAs behavior.

3.1. Description of Device Structures

The devices used in the experiments were modulation-doped field-effect transistor structures without the gate metalization. The advantage of these structures was that they were readily suitable for high-frequency measurements and device-mounting procedures.

A diagram of the gateless MODFET device structure is presented in Fig. 3.1. These MODFET structures were fabricated by Dr. Morkoc of the University of Illinois. The devices are grown on a semi-insulating (SI) GaAs substrate starting with an undoped GaAs buffer layer. This buffer layer is grown to smooth out any defect properties associated with the
Fig. 3.1. Diagram of AlGaAs/GaAs structures.
surface of the SI substrate and to provide a relatively pure GaAs region for electron transport. It also provides a means for obtaining an uninterrupted growth cycle at the AlGaAs/GaAs interface. An undoped AlGaAs spacer layer is incorporated to provide greater separation between the parent donor atoms and the free electrons at the interface. A silicon-doped AlGaAs layer is grown next. The doping level, as well as the spacer layer thickness and conduction-band difference, determine the quasi-two-dimensional electron sheet carrier concentration $n_s$ at the interface. A thin, highly doped n$^+$ cap layer of GaAs is grown to facilitate ohmic contact formation. Source and drain regions are defined by photolithography, and gold is deposited for contact pads.

Details of each structure are found in Table 3.1 for the two wafers numbered 1483 and 1885. Also included are the geometrical width $w$ and length $L$ of each device. The contact resistance $R_c$ associated with the ohmic contact to the active device region is given because of its importance in interpretation of the experimental data.

3.2. Noise Temperature Measurement Setup and Experimental Procedures

Since our investigation is concerned with the determination of the field-dependent diffusion coefficient, the noise component associated with the velocity fluctuations needs to be measured. To measure the velocity fluctuation spectrum, experiments have to be done at frequencies high enough to avoid the g-r and 1/f noise contributions. At high frequencies it becomes difficult to measure the actual terminal voltages and/or currents, so it is easier to measure the available power from the network. This available noise power is related to the noise temperature $T_n$ as described in Chapter I.
### TABLE 3.1
Device Structure Parameters

<table>
<thead>
<tr>
<th></th>
<th>#1483</th>
<th>#1885</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Cap layer thickness (Å)</td>
<td>50</td>
<td>50</td>
</tr>
<tr>
<td>2. Cap layer doping level (cm(^{-3}))</td>
<td>(2.5 \times 10^{18})</td>
<td>(2.5 \times 10^{18})</td>
</tr>
<tr>
<td>3. Doped AlGaAs thickness (Å)</td>
<td>600</td>
<td>350</td>
</tr>
<tr>
<td>4. AlGaAs doping level (cm(^{-3}))</td>
<td>(2.5 \times 10^{18})</td>
<td>(2.5 \times 10^{18})</td>
</tr>
<tr>
<td>5. Aluminum mole fraction (x)</td>
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</tr>
<tr>
<td>6. Undoped spacer thickness (Å)</td>
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</tr>
<tr>
<td>7. GaAs buffer thickness (µm)</td>
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</tr>
<tr>
<td>8. Contact resistance (R_c) (Ω)</td>
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<td>11</td>
</tr>
<tr>
<td>9. Width (w) (µm)</td>
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<td>75</td>
</tr>
<tr>
<td>10. Length (L) (µm)</td>
<td>4</td>
<td>2.8</td>
</tr>
</tbody>
</table>
The technique used to measure the noise temperature of the device under test (DUT) is similar to the method developed by Gasquet et al. [36]. The main advantage of this particular scheme is that it allows measurement of the noise temperature without the need to match the DUT to the characteristic impedance (50 Ω) at each bias and frequency. Not only can matching be a tedious task, but the stub tuners used in matching can have different resistive losses depending on the particular stub settings. The variability of these losses degrades measurement accuracy.

The experimental setup to measure DUT noise temperature over the frequency range 500 MHz to 12 GHz is depicted in Fig. 3.2. This broad range of frequency coverage is obtained by using circulators with octave bandwidths and broad-band low-noise amplifiers. Frequency selection is attained with the spectrum analyzer (HP8559A), which is capable of receiving input frequencies from 10 MHz to 22 GHz. The noise source (HP346B) is also broad-band covering 10 MHz to 18 GHz with an effective noise ratio of 15 dB (T = 9170 K). Amplification and power detection are performed at the intermediate frequency (21.4 MHz) of the spectrum analyzer.

The experimental procedure consists of four measurements to determine the noise temperature $T_n$ of the DUT. These measurements also make available the power reflection coefficient $|\Gamma|^2$ at port 2 of the circulator, the noise temperature $T_a$ of the measuring system, and the gain bandwidth product $GB$ of the system.

The first measurement $M_1$ consists of a reference temperature signal $T_c$ flowing from port 1 in the preferred direction to port 2, where a short-circuit termination is placed. The reference signal is totally
Fig. 3.2. Noise temperature measurement setup.
reflected by this short circuit and proceeds to the amplifier stages at port 3. The amplifier system provides proper impedance termination at port 3. The measured power is then proportional to

$$M_1 = k_B G B(T_a + T_c),$$

where $k_B$ is the Boltzmann constant. The second measurement $M_2$ is essentially the same except that the reference temperature is now $T_h$, giving

$$M_2 = k_B G B(T_a + T_h).$$

Now, the short circuit at port 2 is replaced by the DUT which is biased to the dc voltage of interest. The reflection coefficient between the DUT and circulator is defined in terms of the DUT impedance $Z_{DUT}$ and the characteristic impedance $Z_{00}$ by the relation

$$\Gamma = \frac{Z_{DUT} - Z_{00}}{Z_{DUT} + Z_{00}}.$$  

(3.3)

Since the DUT has, in general, an impedance different from the characteristic impedance of the circulator, the available noise power from the DUT is reduced by the factor $(1 - |\Gamma|^2)$. This property is exploited in the next two measurements.

The noise source temperature is again set to $T_c$ for the third measurement. Since the low-noise amplifier sees a constant impedance looking into port 3 regardless of the impedance change at port 2, the system noise temperature $T_a$ remains the same. Also, the reference temperature is partially reflected at port 2 because of the mismatch, so the measured power is proportional to
\[ M_3 = k_B G B(T_a + T_n(1 - |\Gamma|^2) + T_c|\Gamma|^2) . \]  \hspace{1cm} (3.4)

A final reading is done with the reference temperature at \( T_h \) providing

\[ M_4 = k_B G B(T_a + T_n(1 - |\Gamma|^2) + T_h|\Gamma|^2) . \]  \hspace{1cm} (3.5)

Manipulating these four measurements, one obtains the unknown device noise temperature

\[ T_n = \frac{T_h (M_3 - M_1) + T_c (M_2 - M_4)}{M_3 - M_1 + M_2 - M_4} \]  \hspace{1cm} (3.6)

and the power reflection coefficient as

\[ |\Gamma|^2 = \frac{M_4 - M_3}{M_2 - M_1} . \]  \hspace{1cm} (3.7)

It should be pointed out that the parameters determined by (3.6) and (3.7) are associated with the network connected at the reference plane of port 2 of the circulator. If there are no resistive or radiative losses between the actual DUT and the circulator port, then \( T_n \) is the actual device noise temperature. Any known losses between the DUT and circulator can be easily corrected. Also, the loss between ports 1 and 2 only affect the values of the reference temperatures \( T_c \) and \( T_h \). Correspondingly, the loss between ports 2 and 3 affect only the system noise temperature \( T_a \).

The system noise temperature can be determined from

\[ T_a = \frac{M_1 T_h - M_2 T_c}{M_2 - M_1} , \]  \hspace{1cm} (3.8)

and the gain bandwidth of the system is given by
Another advantage of this measuring technique is that it allows the determination of device noise temperature using either a continuous or pulse bias. When the device is biased into the hot-electron regime, significant Joule heating of the lattice occurs. A pulse bias at low-duty cycle is then required to keep the average power dissipation to a minimum. A pin-diode RF switch is used in the IF section to make sure that only the noise power produced during the bias time is detected. The actual length of bias pulse time is determined by the time constants associated with the bias tee network and the DUT impedance. The bias tee provides the necessary dc and RF isolations.

3.3. Experimental Results

Both device structures used for the measurements were mounted in a 50Ω microstrip transmission line test fixture. The microstrip line was made from a 25-mil.-thick alumina substrate and attached to SMA coaxial connectors. All measurements were made with a covered mount to keep the device in the dark.

The first device to be measured was wafer #1483. Measurements were done with a pulse bias time of 4 ms and a 3% duty cycle at room temperature (300 K). The dc current-voltage characteristic for this 4 μm heterostructure is depicted in Figure 3.3. The low-field equilibrium resistance is found to be 31 ohms. As can be seen in the figure, the I-V characteristic begins to deviate from Ohm's law around 600 mV. This nonlinear behavior is an indication of hot-electron effects in the channel. Changing the polarity of the voltage had no
Fig. 3.3. Current-voltage characteristic of #1483.
effect on the I-V relationship, indicating that the contacts were indeed ohmic and had no rectifying properties.

From the I-V characteristic one can obtain the dc mobility as a function of electric field. The electric field in the channel is assumed to be uniform and found by taking the voltage drop across the active region and dividing it by the length. The definition of dc mobility is given by

\[ \mu(E) = \frac{v(E)}{E} \quad (3.10) \]

Figure 3.4 shows the dc mobility as a function of electric field, normalized to its equilibrium value \( \mu_0 \) after correcting for a contact resistance of 8 ohms. The advantage of normalization is that a better comparison with other heterostructures can be made since it removes any differences in the actual thermal equilibrium mobility values. Also included in the figure are other published experimental results on similar heterostructures [37-39]. Since no other means of obtaining the contact resistance for this structure was available, the value of 8\( \Omega \) was derived by lining up the data with the previously published results in the figure.

Next the noise temperature of #1483 was measured in the frequency range 500 MHz to 1 GHz. No frequency dependence in the noise temperature as a function of bias was observed, indicating the absence of any 1/f or g-r noise components. Therefore, the noise temperature was associated with velocity fluctuations. The actual noise temperature of the active region measured between .5 and 1 GHz and as a function of electric field is displayed in Figure 3.5. It can be seen here how quickly the noise temperature increases for fields far from equilibrium.
Fig. 3.4. Normalized dc mobility as a function of electric field. Circles indicate ungated MODFET #1483, inverted triangles indicate Tsubaki et al. [37], right-side-up triangles indicate Masselink et al. [38], and squares indicate van Welzenis et al. [39].
Fig. 3.5. Noise temperature vs. electric field for #1483.
The differential mobility is obtained from a measurement of the admittance of the DUT. First, the conductance or \( \text{Re}(Y) \) can be calculated from the derivative of the I-V characteristic. This method works well as long as the \( \text{Re}(Y) \) is not frequency dependent in the range of interest. The admittance can also be measured with the use of an S-parameter test set (HP 8410). The drawback of this measurement technique is that it has to be done with a continuous bias. Finally, the magnitude of the reflection coefficient is determined during the noise temperature measurement (3.7). When the susceptive elements are negligible, the \( \text{Re}(Y) \) can be found from the magnitude of the reflection coefficient. Whenever possible, all three methods are combined. For \#1483 all methods showed good agreement in the \( \text{Re}(Y) \) since the parasitic susceptive elements were small compared to the channel conductance.

The diffusion coefficient in the active region of \#1483 can now be determined from the generalized Einstein relation

\[
D(E) = \frac{k_B T_n(E)}{q} \text{Re}(\mu').
\]  

(3.11)

Normalizing the diffusion coefficient to the equilibrium value \( D_0 \), one obtains from the measured data

\[
\frac{D(E)}{D_0} = \frac{T_n(E) \text{Re}(Y)}{T \text{Re}(Y_0)}
\]  

(3.12)

where \( T \) is the lattice temperature and \( Y_0 \) is the equilibrium admittance. A constant carrier concentration in the channel is assumed. The normalized diffusion coefficient as a function of electric field for \#1483 is presented in Figure 3.6. Also included in the figure are the
Fig. 3.6. Normalized diffusion coefficient for #1483 as a function of electric field. Circles indicate ungated MODFET, squares indicate Ruch and Kino [10], inverted triangles indicate Gasquet et al. [25], and the right-side-up triangles indicate Bareikis et al. [24].
normalized diffusion coefficient measurements of bulk GaAs [10,24,25]. It can be seen that the diffusion coefficient of the heterostructure does not increase as significantly as the bulk GaAs results.

Device structure #1885 was measured next. One of the main advantages of this structure was that on the same wafer different-length devices were available for measurement. In this way the contact resistance could be determined more accurately. The low-field ohmic resistance as a function of device length is plotted in Fig. 3.7. The circles indicate the data obtained by using the wafer probe station and the triangles indicate the actual wire bonded values. The discrepancy between the two different measurements is attributed to the contacting problems associated with the wafer probes. However, both sets of data extrapolate to the same value at the origin (L = 0), giving a contact resistance of 110. The current-voltage characteristics of #1885 for lengths of 2 and 8 µm are shown in Figs. 3.8 and 3.9, respectively. Both devices showed hot-electron effects at high bias.

Having the I-V characteristics and the contact resistance, it is again possible to find the dc mobility versus electric field. The normalized dc mobility of #1885 is given in Figure 3.10. There was no difference found in the dc mobility for the two lengths measured. Also, the dc mobility behavior of #1885 is very similar to that of #1483.

Obtaining the Re(Y) from measurements at high frequencies was difficult for this structure. The measured admittance data at low frequencies (f < 500 MHz) showed reasonable behavior, but became quite difficult to model at high frequencies (f > 1 GHz). Because of the large wafer size associated with this structure, very long bonding wires had to be used to make connections to the actual DUT. These long
Fig. 3.7. Resistance vs. length for #1885 to determine contact resistance. Circles indicate wafer-probed values whereas triangles indicate wire-bond values.
Fig. 3.8. Current-voltage characteristic of #1885 (L = 2 μm).
Fig. 3.9. Current-voltage characteristic of #1885 (L = 8 μm).
Fig. 3.10. Normalized dc mobility vs. electric field for \#1885.
bonding wires made it difficult to obtain a good high-frequency ground, and the large wafer may introduce other unaccounted for parasitics. As a result, the Re(Y) of the DUT was determined from dI/dV, and we assumed that it is frequency independent in the range of interest.

The noise temperature of #1885 was measured from .5 to 12 GHz. After accounting for all known losses between the circulator and DUT, the noise temperature showed a slight decrease for frequencies greater than 2 GHz (see Fig. 3.11). This slight decrease was associated with losses in the parasitics that could not be well defined. At other bias values, similar behavior of Tn versus frequency was observed.

Taking the data between .5 and 1 GHz to be accurate, the noise temperature of the active region versus electric field for #1885 is depicted in Fig. 3.12. Again it can be seen that the noise temperature increases with electric field, but not as rapidly as that of #1483.

The normalized diffusion coefficient as a function of electric field is given in Fig. 3.13 for both 2 and 8 μm structures. The Re(Y) is determined from dI/dV. Both device lengths show the same decrease in the diffusion coefficient with field, indicating that there is no noticeable dependence on device length in this range.

3.4. Discussion of Results

In this section we will discuss the hot-electron behavior of the AlGaAs/GaAs interfaces and compare the results to those of bulk GaAs. Only qualitative explanations can be given due to the lack of sufficiently developed analytical models for parallel transport in the heterojunctions or the availability of complex Monte Carlo programs.

Clearly, the first observation that can be made is the similarity in the dc characteristics of different heterointerfaces. The dc
Fig. 3.11. Noise temperature vs. frequency for #1885.
Fig. 3.12. Noise temperature vs. electric field for #1885.
Fig. 3.13. Normalized diffusion coefficient vs. electric field for #1885. Squares and circles indicate 2 and 8 μm data, respectively.
mobility of both #1483 and #1885 decreases with increasing field strength in the hot-electron regime, which also agrees with the previously published results.

However, there does seem to be differences in the noise behavior between different heterointerface compositions. For device #1483 the diffusion coefficient (or velocity fluctuation spectral density) remains nearly constant with increasing field, whereas #1885 shows a slight decrease in the hot-electron regime. This difference in diffusion coefficients results mainly from the lower noise temperature measured in #1885.

Both heterojunction interface structures show a clearly different noise behavior than bulk GaAs. In bulk, the increase in the diffusion coefficient with field was attributed to polar runaway and intervalley transfer (sec. 2.2). A decrease in the importance of one or both of these mechanisms in the heterointerfaces might be responsible for the observed D(E) dependence. Differences due to device length are not suspected since no noticeable length dependence of D(E) is observed in the diffusion coefficient measurements of the 2 and 8 μm channels of #1885 presented in Fig. 3.13.

Yokoyama and Hess [40] calculate the two-dimensional scattering rates for electrons in the first five subbands of a quasi-triangular potential well at the AlGaAs/GaAs interface. Their results show lower scattering rates for polar optical phonons as compared to the rates for bulk GaAs at room temperature. Since the polar-optical phonon scattering rates are reduced in two-dimensional systems, the effects of the polar runaway phenomenon may be less significant.
The second contributing factor to the diffusion coefficient in bulk GaAs is intervalley transfer. In the case of interfaces, this process is difficult to model because of the real-space-charge transfer from the GaAs to the AlGaAs. An electron might cross the energy barrier at the interface before gaining enough energy to undergo intervalley transfer. Indeed, the conduction-band difference at the interface is smaller for device #1885 by 40 meV, which is the structure that shows the decreasing diffusion coefficient with electric field. Since there is a lack of experimental data on the AlGaAs system, it is very difficult to model or otherwise evaluate hot-electron properties in this region or its effect on real-space-charge transfer.

The only analytical support for the diffusion coefficient behavior in the heterointerfaces is from the Monte Carlo model of van Rheenen and Bosman [41]. In their model they use an infinitely high, square potential well to simulate the two-dimensional transport behavior of a two-valley GaAs channel. The diffusion coefficient in this simulation shows a decrease with increasing electric field as opposed to the increase in diffusion observed in their bulk simulation. Therefore, the decrease in the diffusion coefficient with increasing field in the heterostructures is possibly linked to the two-dimensionality of the electron gas.
In recent years much attention has been paid to AlGaAs/GaAs modulation-doped field-effect transistors (MODFETs) for potential use in high-speed logic circuits. The very high transconductance $g_m$ and high cut-off frequencies $f_T$ also make them of interest for low-noise microwave amplification. Excellent articles by Solomon and Morkoc [2] and Drummond et al. [42] have been written reviewing the characteristics of these new transistors.

Since the first report of the noise figure of these devices in the microwave frequency range, an interest in the noise behavior has developed. The noise figures of various MODFETs have been reported recently and show improvements over conventional GaAs MESFETs of comparable gate lengths.

Up to now only noise-figure measurements have been reported in the microwave frequency range. In this chapter we will not focus on the noise figure, but instead report on the noise characteristics of the FET channel. At intermediate frequencies ($0.5 < f < 10$ GHz) the channel noise is due to fluctuations of the free-carrier velocity and is the major contributor to the overall device noise. Measurements of the thermal noise (i.e. velocity fluctuation noise) as a function of bias are discussed in this chapter.

In section 4.1 we will outline the theory of the impedance field method, which is used to obtain the ac and noise properties of the MODFET channel. Section 4.2 explains the methods of obtaining the charge-voltage relationship for the devices used in our experiments. Some of the methods of obtaining the charge-voltage relationship involve
only low-bias data while other methods involve high-bias data. Comparing the results of the different methods can help determine the presence or absence of real-space-charge transfer. Section 4.3 describes the MODFET structures to be considered. Measurement procedures are discussed in section 4.4. The experimental results will then be presented and discussed in section 4.5, followed by conclusions in section 4.6.

4.1. Impedance Field Modeling

In this section the procedure for obtaining the position-dependent ac channel voltage in terms of the Green's function for a MODFET channel is discussed. It will be shown how the Green's function is related to the impedance field [16,17]. Once the impedance field is obtained, the ac and noise properties can be easily calculated. Van Vliet [43] and Nougier [44] have outlined this method for the case of the junction field-effect transistor (JFET). In this chapter the impedance field for a MODFET is calculated using the proper transport equations, and the ac and noise properties of the MODFET are derived.

4.1.1. Review of impedance field method

The procedure begins by considering the device transport equations. Small-signal variations around the steady-state values of all of the variables are introduced. Having done this, and neglecting second-order and higher terms, the ac and dc equations can be separated. The dc equation can be used to obtain the steady-state current-voltage characteristic of the device.

The ac equation has some interesting properties. Generally, the ac equation involves the position-dependent steady-state parameters. This equation can be written as follows:

\[ \hat{N}A\hat{V}(x) = \Delta I(x) \] (4.1)
where \( \hat{H} \) is a linear operator and \( \Delta V \) and \( \Delta I \) are the small-signal ac channel voltage and current respectively. By letting \( z(x,x',f) \) be the Green's function of \( \hat{H} \), i.e.
\[
\hat{H}z(x,x',f) = \delta(x-x'),
\]
(4.2)
where \( \delta(x-x') \) is the Dirac delta function and \( f \) denotes frequency, the total ac voltage at position \( x \) can be calculated from
\[
\Delta V_T(x) = \int_0^L z(x,x',f)\Delta I(x')dx'.
\]
(4.3)
The integration is taken over the entire length of the device. The total ac voltage at \( x \) given by eq. (4.3) is simply the summation over all of the small-signal current sources properly weighted by the terms \( z(x,x',f)dx' \). Depending on the charge transport mechanisms involved, some of the terms \( z(x,x',f) \) might be zero. This point will be illustrated when the equations are developed for the MODFET. Of course, one is mainly interested in the values of the small-signal quantities at the device terminals, since these can be measured. The total small signal voltage at the device terminal (\( x = L \)) is
\[
\Delta V_T(L) = \int_0^L z(L,x',f)\Delta I(x')dx'.
\]
(4.4)
The one-dimensional device shown in Fig. 4.1 is grounded at \( x = 0 \) and has an arbitrary steady-state dc bias applied at \( x = L \). Suppose a current of value \( \Delta I(x) \) is introduced at position \( x + \Delta x \) and extracted at \( x \). \( \Delta I(x) \) will produce an open-circuit voltage response \( \Delta V(L) \) at the terminal (\( x = L \)). If the ac impedance between position \( x \) and ground (\( x = 0 \)) is given by \( Z(x) \), then the voltage response at \( L \) can be expressed as
Fig. 4.1. A small signal current $\Delta I(x)$ produces a voltage response $\Delta V(L)$ at the terminal $x = L$. Steady-dc current $I_0$ and voltage $V_0$ are indicated.
\[ \Delta V(L) = [Z(x+\Delta x, f) - Z(x, f)] \Delta I(x) . \quad (4.5) \]

For small \( \Delta x \)

\[ Z(x+\Delta x, f) = Z(x, f) + \frac{dZ(x, f)}{dx} \Delta x , \quad (4.6) \]

and one obtains

\[ \Delta V(L) = VZ(x, f) \Delta I(x) \Delta x . \quad (4.7) \]

The term \( VZ(x, f) \) is known as the impedance field and was first introduced by Shockley et al. [16]. The impedance field relates the ac current inside the device to the voltage response at the terminals. In the limit \( \Delta x \rightarrow dx \) the total ac voltage at \( L \) is given by

\[ \Delta V_T(L) = \int_0^L VZ(x', f) \Delta I(x') dx' . \quad (4.8) \]

Comparing eqs. (4.8) and (4.4), one sees that

\[ VZ(x', f) = z(L, x', f) . \quad (4.9) \]

To find the total device impedance at the terminals, one makes use of the fact that the ac current is conserved. Then \( \Delta I(x) = \Delta I \), and consequently

\[ Z(L) = \frac{\Delta V_T(L)}{\Delta I} = \int_0^L VZ(x', f) dx' = \int_0^L z(L, x', f) dx' . \quad (4.10) \]

Using the impedance field, one can express the noise in terms of spectral densities. The spectral density of the open-circuit voltage fluctuations measured at the terminals is given by [16]

\[ S_{\Delta V} = \iint_0^L K(x')|VZ(x', f)|^2 dx' dy dz \quad (4.11) \]
where \( K(x') \) is the spectral density of the current fluctuations in volume \( dx'dydz \), and the integration is carried out over the entire volume of the device. Using eq. (4.11), the spectral density of 1/f noise, generation-recombination (g-r) noise, and velocity-fluctuation noise can be calculated if the proper source term \( K(x') \) is inserted.

In this chapter the focus is on velocity-fluctuation noise only. It has been shown in Chapter I that the spectral density of velocity fluctuations is directly related to the diffusion coefficient \( D(E) \), which may be field dependent. Taking this effect into account, Nougier shows that the spectral density of the voltage fluctuations due to velocity fluctuations in a one-dimensional treatment becomes [44]

\[
S_{\Delta V} = \int_0^L A(x') 4q^2 D[E(x')] n(x') \left| \nabla Z(x',f) \right|^2 dx'
\]

(4.12)

where \( A(x') \) is the cross-sectional area, \( n(x') \) is the carrier density and \(-q\) is the electron charge. The equivalent current-noise spectral density \( S_{\Delta I} \) can be calculated from

\[
S_{\Delta I} = \frac{S_{\Delta V}}{|Z(L)|^2}.
\]

(4.13)

4.1.2. Application of the impedance field method to the MODFET

In the following a one-dimensional, collision-dominated transport model is used to obtain simple analytical expressions for the impedance and noise of the device. The advantage of this approach is that it provides physical insight into the ac and noise behavior of the channel. Clearly this treatment breaks down for very short submicron devices \((L < .5 \mu m)\) since in that case the usual concept of mobility and diffusion needs to be generalized (see Constant [45]). Assuming no leakage
current through the gate and neglecting both diffusion and displacement currents, the charge transport equation is given by

$$I = qwn_s[V(x)]v[E(x)],$$

(4.14)

where $w$ is the gate width and $v[E(x)]$ is the field-dependent carrier velocity. The sign convention is as follows. The source is chosen at $x = 0$, the drain at $x = L > 0$, $q > 0$, $V(x) > 0$, $E(x) < 0$, $v[E(x)] > 0$, and $I > 0$. The two-dimensional sheet carrier concentration $n_s[V(x)]$ is assumed to be only a function of the local electrical potential under the gate. Velocity saturation will cause accumulation and/or depletion of the sheet carrier concentration in the high-field region under the gate, making eq. (4.14) invalid. For this reason the model we employ only describes the linear and triode regimes of the current-voltage characteristic. At $T = 300$ K the velocity-field characteristic of the two-dimensional electron gas is assumed to be identical to the one of bulk GaAs [46]. Consequently,

$$v(E) = \frac{-\mu_0 E}{1 - E/E_c}$$

(4.15)

where $\mu_0$ is the low-field mobility taken to be $8000 \text{ cm}^2/\text{V sec}$ at room temperature, and the critical field $E_c$ is chosen to be $11.4 \text{ kV/cm}$. When the electric field exceeds $3.5 \text{ kV/cm}$, the model [eq. (4.14)] no longer holds due to the saturation effects mentioned above. The large critical field $E_c$ is chosen to provide the proper curvature of the velocity characteristic at low electric fields. Using the bulk GaAs velocity-field characteristic as a first attempt is justified since in the high-field region under the gate the reduced sheet carrier concentration
causes the quasi-triangular potential well to widen. As the well widens, the electron gas goes from quasi-two-dimensional to three-dimensional bulk. This phenomenon is confirmed by the results of Monte Carlo simulations by Cappy et al. [46]. In addition, Cappy observed that real-space-charge transfer of hot carriers from the interface back to the AlGaAs layer can be neglected in a MODFET.

The ac and dc transport equations are obtained by linearizing eq. (4.14) in the following way. Introducing small-signal variations around the steady-state quantities, one obtains

\[ I = I_0 + \Delta I \] (4.16)

\[ n_s(V) = n_s(V_0) + \left( \frac{dn_s}{dV} \right)_0 \Delta V \] (4.17)

\[ v(E) = v(E_0) + \left( \frac{dv}{dE} \right)_0 \Delta E . \] (4.18)

Substituting (4.16), (4.17) and (4.18) into (4.14), the expression for the dc current becomes

\[ I_0 = -qw_n [V_0(x)] \mu_0 E(x)/(1 - E(x)/E_c) \] (4.19)

and for the ac current, after neglecting second-order terms and using \( \Delta E = -d\Delta V/dx \), one finds

\[ \Delta I(x) = -qw_n [V_0(x)] \left[ \frac{dv}{dE} \right]_0 \frac{d\Delta V(x)}{dx} + qw \left( \frac{dn_s}{dV} \right)_0 v(E_0) \Delta V(x) . \] (4.20)

Equation (4.20) relates the ac current and voltage at position \( x \) by a first-order differential equation. An analytical solution is easily obtained by rearranging eq. (4.20) to the form
\[
\frac{dy}{dx} + P(x)y = Q(x),
\]

(4.21)

which has the solution

\[
y = \exp \int P(x)dx \left[ \int \exp \int P(x)dx Q(x)dx + c \right].
\]

(4.22)

Since the source end of the MODFET is grounded, \( \Delta V(0) = 0 \) and the integration constant vanish. Consequently, one obtains

\[
\Delta V(x) = \frac{H(x-x') (1 - \frac{E_0(x')}{E_c})\Delta I(x')}{qw_0 n_s [V_0(x')] - I_0/E_c}
\]

\[
\exp \int_{x'}^{x} \frac{\exp \int_{0,u}^{s} dV \frac{d\mu}{dV}}{qw_0 n_s [V_0(u)] - I_0/E_c} du
\]

(4.23)

where \( H(x-x') \) is the unit step function. Upon integration of the exponential term, eq. (4.23) simplifies to

\[
z(x,x',t) = \frac{H(x-x') (1 - \frac{E_0(x')}{E_c})}{qw_0 n_s [V_0(x)] - I_0/E_c}.
\]

(4.24)

The unit step function has the physical significance that the ac voltage at position \( x \) only depends on the ac current variations introduced between the source \( (x = 0) \) and position \( x \). Hence ac current variations only propagate a voltage response toward the drain end of the device. This arises because the conduction in a MODFET is dominated by drift. If diffusion had a significant effect on current flow and had to be included, the ac transport equation would become second order. Then the voltage response of \( \Delta I(x) \) would propagate to the drain as well as to the source terminal of the device. This effect was found in short, space-charge-limited diodes by Tehrani et al. [18].
To obtain the impedance field from (4.24), one substitutes \( x = L \) and finds

\[
z(L,x',f) = \frac{-E_0(L)}{I_0} \left(1 - \frac{E_0(x')}{E_c}\right). \tag{4.25}
\]

Then, with the help of eq. (4.10), one derives for the device impedance

\[
Z(L) = \frac{-E_0(L)L}{I_0} \left(1 + \frac{V(L)}{E_c}\right) \tag{4.26}
\]

where \( V(L) \) is the dc voltage at \( L \).

Having obtained the impedance field and device impedance for the MODFET, the expressions for the noise can be calculated. The spectral density of the open-circuit-voltage noise, using (4.25) and (4.12), becomes

\[
S_{\Delta V} = \int_0^L \frac{dE(x')}{dE} \frac{q^2}{D(E(x'))} \frac{E_0(L)}{I_0} \left(1 - \frac{E_0(x')}{E_c}\right)^2 \, dx'.
\tag{4.27}
\]

The spectral density of the current noise can easily be found from eqs. (4.13) and (4.26).

Often the expressions for the noise of a device are given in terms of an ac noise temperature \( T_n(E) \). With the help of the generalized Einstein relation

\[
D(E) = \frac{k_B T_n(E)}{q} \mu'(E), \tag{4.28}
\]

where \( k_B \) is Boltzmann's constant, \( \mu'(E) \) is the differential mobility, i.e., the derivative of the velocity-field characteristic at a given
field, one gets

\[ S_{\Delta V} = \left( \frac{E_0(L)}{L_0} \right)^2 \frac{4q\mu_0 wk_B}{L^2} \int_0^L T_n[E(x')] n_s[V_0(x')] dx' \]  

(4.29)

and

\[ S_{\Delta I} = \left( \frac{V(L)}{E_c L} \right)^2 \frac{4q\mu_0 wk_B}{(1 + \frac{V(L)}{E_c L})^2} \int_0^L T_n[E(x')] n_s[V_0(x')] dx' \]  

(4.30)

for the spectral densities of the voltage and current noise, respectively.

4.2. Charge-Voltage Dependence

To successfully use the expressions for the impedance and noise in the case of a MODFET, the proper relationship between the sheet carrier concentration and the electrical potential in the channel has to be known. Several authors [47,48] used an effective capacitance and threshold voltage to calculate \( n_s(V) \) as is usually done in a MOSFET. In addition they assumed a constant mobility up to saturation. Good agreement between experimental and theoretical I-V characteristics was found for some enhancement-mode devices. Also, the thermal noise was calculated using these models [49]. However, our experimental findings could not be explained using these models.

Solving the Poisson and Schrödinger equations self-consistently, Vinter [50] shows that for the MODFET structures he considers that the gate capacitance depends strongly on gate bias. This gate bias dependence of the capacitance can be observed experimentally in the transconductance measurements of Gupta et al. [51].

There are several experimental methods for obtaining the correct charge-voltage dependence. In the first method the small-signal gate-
to-channel capacitance is measured as a function of gate bias. This capacitance is proportional to the derivative of the charge-voltage relationship. In addition, a measurement of the low drain bias ($V_{DS} << 50 \text{ mV}$) total channel resistance as a function of $V_G$ is required. This resistance is given by

$$R_{DS}(V_G) = R_{ss} + R_{dd} + \frac{L}{qwu_0n_s(V_G)}$$

where $R_{ss}$ and $R_{dd}$ are the source and drain access resistances respectively and $L$ is the gate length. The last term in (4.31) accounts for the resistance of the channel region under the gate. Taking the derivative of (4.31) with respect to $V_G$, one obtains

$$\frac{dR_{DS}(V_G)}{dV_G} = \frac{-L(dn_s)}{qwu_0n_s^2(V_G)}.$$  

(4.32)

It is clear from eq. (4.32) and the capacitance measurements that one has enough information to obtain the charge-voltage relationship without the knowledge of the access resistances $R_{ss}$ and $R_{dd}$.

Direct measurements of the gate capacitance on small geometry MODFETs ($L < 1 \text{ \mu m}$) may prove to be difficult and/or inaccurate because of parasitic effects. If one has large area devices fabricated on the same wafer, measurements of this sort could be done.

A second, approximate method is to use eq. (4.31) and estimate the value of $R_{ss} + R_{dd}$. The charge-voltage relationship is then directly obtainable without knowledge of the capacitance. Estimates of the value of $R_{ss} + R_{dd}$ can be made with the help of calculations for heterojunction lineup in equilibrium [52] and the quasi-triangular potential-well approximation. These calculations are expected to give sheet carrier
concentrations of reasonable enough accuracy to obtain the end resistances.

Finally, a third method is introduced to obtain the charge-voltage relationship. It involves the small-signal impedance of the channel for any value of drain bias for which the impedance field model outlined earlier holds.

Position $L_1$ (see Fig. 4.2) is the point taken to be the drain-side edge under the gate. At this point the maximum electric field in the channel is produced. Its value is not allowed to exceed the peak field value of 3.5 kV/cm in our impedance field model. The charge at $L_1$ is controlled by the gate voltage. The impedance at $L_1$ is given by [c.f. eq. (4.26)]

$$Z(L_1) = \frac{-E_0(L_1)l_1}{\frac{1}{I_0} (1 + \frac{V(L_1)}{E_c L_1})}.$$  \hspace{1cm} (4.33)

With reasonable knowledge of the drain resistance $R_{dd}$, then, this impedance is

$$Z(L_1) = Z(L) - R_{dd}$$ \hspace{1cm} (4.34)

and the dc voltage at $L_1$ is

$$V(L_1) = V_{DS} - I_0 R_{dd}.$$ \hspace{1cm} (4.35)

Then from eq. (4.33) a value for $E_0(L_1)$ can be calculated using the measured current- and impedance-voltage characteristics, and the sheet carrier concentration at $L_1$ follows from eq. (4.19). In this way the charge-voltage relationship is obtained in the presence of high electric fields under the gate. If this method gives results for $n_s(V)$ similar
Fig. 4.2. Diagram of the MODFET structures used in our experiments.
to the other two methods, which are based on the assumption that the field under the gate is low, then the absence of real-space-charge transfer in MODFET operation is experimentally verified.

Note that all of the above methods are restricted to the regime of operation where the AlGaAs layer under the gate is fully depleted of carriers. Also, it is assumed that the two-dimensional sheet carrier mobility is not a function of gate bias.

4.3. Device Description

A diagram of the MODFET structure used in our measurements is shown in Fig. 4.2. The gate is recessed so that the space-charge regions of the Schottky barrier and the AlGaAs/GaAs interface overlap. The gate-interface spacing determines whether the device will operate in the enhancement or depletion mode. Experiments were performed on two depletion mode MODFETs with a gate length of 1 μm and a gate width of 145 μm. Spacing between the source and drain pads was 4 μm. Regions I and III represent the source and drain access resistances $R_{SS}$ and $R_{dd}$, whereas Region II is the active gate region.

In the case of device #1483, a GaAs buffer layer of 1 μm thickness was deposited on a GaAs semi-insulating substrate. Next a 30 Å intrinsic AlGaAs spacer layer with an aluminum mole fraction $x = 0.28$ was grown on top, followed by a 600 Å layer of AlGaAs doped to a level of $2.5 \times 10^{18} \text{ cm}^{-3}$. The second device (#2010) measured had a 1 μm-thick GaAs buffer layer, 30 Å spacer layer with aluminum mole fraction $x = 0.20$, followed by a 350 Å layer doped to $5 \times 10^{18} \text{ cm}^{-3}$.

4.4. Measurement Procedure

Measurements of the current-voltage characteristics of the MODFET structures show that device #1483 exhibits a significant change in the
current with time for a fixed bias voltage. For this device the current could be stabilize when the drain bias was pulsed with a low-duty cycle. This indicates that the current change was due to Joule heating of the channel. In our setup a pulse length of four milliseconds at a three percent duty cycle was used. Shorter pulses could not be applied due to the rise time of the bias tee. Under these conditions the I-V characteristic of each device was measured from the linear region up into saturation using a digital oscilloscope.

The noise measurement scheme is shown in Fig. 4.3 and is a modified version of the setup described in Chapter III. From a series of four measurements at each bias setting, the noise temperature $T_n$ of the device under test (DUT), the power reflection coefficient $|r|^2$ at port 2 of the circulator, the noise temperature of the amplifier system $T_a$, and the gain bandwidth product of the system can be obtained. All losses, including any mismatch of the DUT, are accounted for in this way.

Each MODFET was measured in the common source configuration with the gate high frequency short-circuited to ground. This is done to eliminate the contribution from the equivalent current-noise source associated with the gate of the device. At a gate bias of $V_G = 0$ V a small bonding wire located very close to the gate is used to short-circuit the input. At high frequencies, when the inductive reactance of the wire becomes too large to effectively short the gate, a high-quality shorted coaxial phase shifter is placed in parallel with the gate. The length of this shorted transmission line can be adjusted to produce an electrical short circuit at the physical gate of the device. By adjusting the phase shifter a minimum in the noise temperature of the DUT at a given frequency could be observed. The minimum corresponds with the
Fig. 4.3. Noise measurement setup for continuous or pulse bias conditions.
condition of a high-frequency shorted gate. This, and the measurement of a white noise spectrum, indicate that the gate current-noise source has been completely canceled. When measuring the noise at gate biases other than \( V_G = 0 \) V, the phase shifter by itself proved to be adequate to cancel the gate noise contribution.

The output of the DUT can be matched at each bias point with the tuner to the characteristic impedance (50 ohms) of the system. The noise generator is used as a calibration noise source as well as for the purpose of matching the DUT. A circulator is used to couple both the device noise and the calibration noise generator to the amplifier stages. The contribution from the noise generator, seen by the amplifier stages, depends on the reflection coefficient seen at port 2 of the circulator. Since the impedance levels of the MODFET channel, from the linear to saturation regimes, do not cause large mismatches from the characteristic impedance, the tuner is not always needed. Measurements of \( T_n \) obtained with and without the tuner agreed well within the experimental error. If the tuner is omitted, the channel reflection coefficient and the noise can be measured simultaneously.

Using broadband circulators and amplifiers, a frequency range from 500 MHz to 3.4 GHz could be covered. A range of frequencies needs to be measured to determine whether the noise spectrum is indeed white. Frequency selection is obtained from the spectrum analyzer which shifts the high-frequency noise signal to an intermediate frequency (IF) of 21.4 MHz. At this frequency further amplification and power detection are performed. This system has the advantage that the noise of the DUT can be measured under continuous or pulse bias. If the measurement is done under pulse bias, the RF switch and the pulse bias generator are
synchronized so that only noise generated during the bias pulse is measured.

Once the ac noise temperature $T_n$ is known, the DUT equivalent current-noise spectral density is obtained from

$$S_{\Delta I}(f) = 4kT_n \text{Re}(Y)$$

(4.36)

where $\text{Re}(Y)$ is the real part of the small-signal admittance of the DUT. The value of $\text{Re}(Y)$ was obtained in the three different ways outlined in Chapter III.

4.5. Results and Discussion

In this section the experimental results obtained on device #1483 will be discussed first, followed by a discussion of the results obtained on device #2010.

The current-voltage characteristic of device #1483 at room temperature with gate bias $V_G = 0$ V is shown in Fig. 4.4. The spectral densities of the open-circuit voltage and short-circuit current noise as a function of the dc current are depicted in Fig. 4.5. The solid lines in both figures indicate the results of the impedance field model outlined in the text. The model is valid up to 26 mA, because at this current value the peak electric field in the channel reaches 3.5 kV/cm. The continued increase in the measured I-V characteristic beyond 26 mA is due to the formation of an accumulation layer under the drain side of the gate. A large voltage drop will occur across this accumulation layer, leading to current saturation in analogy with the situation in GaAs MESFETs [33].

The charge-voltage relationship used in our calculations was derived by using the measured ac impedance and I-V characteristic
Fig. 4.4. Current-voltage characteristic of #1483 at $V_G = 0$ V. The black dots present the experimental data. The solid line indicates the results of our model and the dashed line indicates the results of the constant capacitance and mobility model.
Fig. 4.5. Voltage and current noise spectral densities as a function of dc current $I_0$. The solid line indicates the results of the impedance field model outlined in the text using $D(E) = D_0$. The dashed line indicates the results of the constant capacitance and mobility model.
A drain resistance $R_d = 6.2$ ohms was used. This value results from equilibrium calculations for heterojunction lineup.

Although calculations and measurements [24,25] show that the diffusion coefficient begins to increase near $3.5$ kV/cm for bulk GaAs, we assume that $D(E) = D_0$. Also, measurements of the diffusion coefficient on gateless MODFET structures shown in Chapter III do not increase with field as in bulk, further justifying our assumption.

The dashed lines in Figs. 4.4 and 4.5 are the predicted performance curves of a MODFET using the constant capacitance and mobility models previously mentioned. Although the calculated current noise spectral density in Fig. 4.5 shows good agreement with experiment, the voltage spectral density does not. This is due to the fact that these models do not correctly predict the small-signal impedance levels in this region of operation, as can be seen in the I-V characteristic of Fig. 4.4.

An attempt was made to measure this same device at liquid-nitrogen temperature. A collapse of the I-V characteristic was observed, similar to what other researchers found at low temperatures [53]. This behavior has been associated with the presence of deep-level traps in the AlGaAs layer. This collapse can be avoided by placing a light-emitting diode (LED) close to the MODFET to empty these traps. However, this method is not suitable in noise measurements, since the LED may cause changes in the noise temperature of the electron gas.

After returning the device to room temperature, the static I-V characteristic had changed, giving a lower saturation current and higher resistance in the linear regime. Since the device had not been hermetically sealed when lowered into the liquid-nitrogen bath, the number of
surface states in regions I and III might have been changed, modulating the width of the surface and AlGaAs/GaAs interface depletion regions, and hence $R_{ss}$ and $R_{dd}$. This would result in an increase in the access resistances and account for the lower saturation current. It is assumed that the gate metallization protected the surface in region II. This seems to be justified by the measurements of the transconductance and charge-voltage relationship both before and after cooling.

The I-V characteristic and noise at $T = 300$ K after a cooling cycle are shown in Figs. 4.6 and 4.7, respectively. There is little change in the behavior of the noise characteristics. Since the total channel resistance has changed, the levels of the noise are slightly different. Our model again shows good agreement with experiment.

Shown in Fig. 4.8 are the results for the charge-voltage relationship obtained using two different methods. The triangles indicate the results for $n_s(V_G)$ calculated using method III with an increased drain resistance of 9.7 ohms after cooling. The circles represent the values determined with the help of method II with $R_{ss} + R_{dd} = 2 \times R_{dd} = 19.4$ ohms. The charge-voltage dependence, choosing slightly different total access resistances equal to 20.9 ohms, is indicated by the squares. Note that method III involves high-field regions under the gate, while method II assumes a low-field, ohmic regime under the gate. From the fact that both methods give identical results for $n_s$, we conclude that the velocity-field curve used in our model correctly describes the charge transport under the gate and, secondly, that real-space-charge transfer in the gate region of a MODFET is absent.

Measurements of the I-V characteristic and the spectral density of the current noise in device #2010 are shown in Figs. 4.9 and 4.10,
Fig. 4.6. Current-voltage characteristic of #1483 at $V_G = 0$ V and $T = 300$ K after cooling cycle.
Fig. 4.7. Voltage and current noise spectral densities as a function of dc current $I_0$ for #1483 at $V_G = 0$ V and $T = 300$ K after cooling cycle.
Fig. 4.8. Charge-voltage relationship of device #1483. The circles and squares indicate data obtained with method II (low field) using $R_{ss} + R_{dd} = 19.4$ and 20.9 ohms respectively. Triangles indicate method III (high field) with $R_{dd} = 9.7$ ohms.
respectively, and were done at the gate bias of maximum transconductance $V_C = -2.5 \text{ V}$. Note the lack of strong current saturation at higher bias. Measurements of the reflection coefficient $\Gamma$ and S-parameter data indicate that the real part of the output admittance varies strongly with frequency. The measured spectral density of the current noise of device #2010 shows a frequency-dependent behavior, indicating that generation-recombination (g-r) noise masks the thermal noise in this frequency range. The maximum transconductance of #2010 was 73.1 mS/mm which is rather low for a MODFET at room temperature. The poor transconductance, the frequency dependence of the channel conductance and the large amount of g-r noise indicate that the interface trap concentration in device #2010 is very high and dominates the charge-transport mechanism.

4.6. Conclusions

This chapter has reviewed the method for obtaining the dc, ac and noise properties of an active semiconductor device based on the impedance field. The impedance field was then derived for the MODFET channel. Calculations using the impedance field model show excellent agreement with measurements. Methods of obtaining the correct charge-voltage relationship under the gate region are examined. The charge-voltage relationship obtained with low and high fields in the channel show excellent agreement, indicating that real-space-charge transfer is not present in the bias range up to saturation. Also, it was shown that poor interface growth strongly affects the noise in the channel of MODFETs.
Fig. 4.9. Current-voltage characteristics of device #2010 at gate bias $V_G = -2.5$ V and $T = 300$ K.
Fig. 4.10. Measured spectral density of the current noise as a function of dc current. Squares indicate data obtained at 500 MHz while circles indicate data obtained at 1 GHz.
5.1. Monte Carlo Transport Modeling

In Chapter II the methods for Monte Carlo modeling of electron transport were reviewed. The computer program was written in such a way that all three conduction-band valleys of GaAs were included, leading to an accurate model of the hot-electron transport regime of GaAs. Improvements in the band-structure model can be made by including the nonparabolicity factor of each valley.

The electron velocity component along the direction of the applied electric field is sampled for a time-series analysis. This procedure only allows the longitudinal diffusion coefficient to be simulated for GaAs. It would be a simple modification to the program to monitor the perpendicular velocity components to simulate the transverse diffusion coefficients. The transverse diffusion coefficients might also show specific electric field or frequency dependences as does the longitudinal characteristics.

With the addition of monitoring the transverse velocity components, one could obtain the electron position in the plane, perpendicular to the field direction. Then real-space-charge transfer between the GaAs and AlGaAs regions could be simulated. The main problem at this point, however, is the lack of sufficient information on the AlGaAs alloy system to properly model the high-field transport properties in
this region. Further experimental research of AlGaAs properties could possibly shed some light on this much utilized alloy.

Other scattering mechanisms can also be included in the program. Impurity scattering can be incorporated with the techniques outlined by Boardman [20] to improve the results at low temperatures. Also, electron-electron interactions may have a significant effect on the electron distribution function in heavily doped material.

For short channel devices, the effects of space charge near the injecting and collecting contacts can be included. This would give better predictions of the noise behavior of short-length active regions in $n^+\!-\!n\!-\!n^+$ structures. It may also lead to electron injection structures tailored to improve noise and speed characteristics.

5.2. Experimental Characterization of Heterostructures

As can be seen from the results presented in Chapter III, the dc characteristics of various heterostructures in the hot-electron regime are very similar. Only when the diffusion coefficients are investigated do the differences in the transport behavior become noticeable. There is clearly a difference between the hot-electron diffusion coefficient of electrons in bulk GaAs and of electrons in heterointerfaces. The main problem in the interpretation of these measurements lies in the complexity of the different physical mechanisms involved.

To further investigate the transport properties of electrons at heterointerfaces, it would be easier for interpretation to suppress the real-space-charge-transfer mechanism as much as possible. Only recently has it become possible to obtain good interfaces with other compound semiconductors with larger conduction-band offsets such as the AlGaAs/InGaAs heterojunction. By making square or triangular quantum-well
interfaces and reducing the real-space-charge transfer, it might become possible to obtain some experimental evidence of the two-dimensional effects on the diffusion coefficient. Of course it is required, for comparison, to determine also the bulk properties of the alloy systems (AlGaAs, InGaAs, etc.) in which electron transport occurs.

5.3. MODFET Characterization

Chapter IV highlighted the impedance field technique and how to apply the method to the modeling of the modulation-doped field-effect transistor (MODFET). The model was based on a collision-dominated, macroscopic treatment of the transport parameters in the active channel region. Good results between the theoretical and experimental dc, ac and noise properties were obtained.

Extensions can be made experimentally in the determination and characterization of the current noise observed at the gate terminal which profoundly affects the high-frequency noise figure. Also, comparative studies of the noise properties between different MODFET interface compositions and conventional MESFETs might provide insight into the physical mechanisms responsible for the improvement in the noise figure observed in MODFETs, which are presently unknown.

For the area of modeling, improvements can be made in the case of very short gate-length devices. Here the collision-dominated models used in Chapter IV break down and a more microscopic approach may be necessary. The assumption that the velocity fluctuations are uncorrelated in space when the active device length becomes comparable to the mean free path requires further consideration.
APPENDIX A
MONTE CARLO ELECTRON TRANSPORT ALGORITHM
APPENDIX B
VELOCITY TIME SERIES ALGORITHM

GEN FLIGHT TIME

IS FLIGHT TIME LONG ENOUGH TO SAMPLE

N

TIMEX = TIMEX + TIME
GO SCATTER

Y

ADVANCE AND SAMPLE VELOCITY

DETERMINE NUMBER OF SAMPLES IN REMAINING TIME NN

Y

NN ≠ 0

ADJUST TIMEX GO SCATTER

N

UPDATE SERIES NN TIMES

ADJUST TIMEX GO SCATTER
APPENDIX C
POSITION-MONITORING ALGORITHM

Z=0
GENERATE VELOCITY FROM MODIFIED MAXWELLIAN

GENERATE FLIGHT TIME

INITIAL VELOCITY LESS THAN 0

Y

CALCULATE TMIN

N

THETA LESS THAN TIME

N

CALCULATE ZMIN

Y

ZMIN LESS THAN 0

N

UPDATE TIME SERIES IFLAG=2

Z LESS THAN L

Y

UPDATE TIME SERIES IFLAG=1

UPDATE TIME SERIES GO SCATTER

123
APPENDIX D

MONTE CARLO COMPUTER PROGRAM
COMPUTER SIMULATION OF THE DIFFUSION COEFFICIENT AND VELOCITY FLUCTUATION SPECTRUM OF ELECTRONS IN SHORT LENGTH GAAS DEVICES

DOUBLE PRECISION

M, NO, NB, NI, KZTOT, VAVG, V2AVG, V3AVG, V4AVG, DIF

DOUBLE PRECISION

NE, NI, KZTOT, TIM1, TIM2, TIM3, MAXE

DOUBLE PRECISION

B, Z, ZIN, TMIN, LGTH, ACCEL

DOUBLE PRECISION

F(10), GAMMA(3), EF(18), SCATT(18)

INTEGER

NF, VR, TT, V, SR, SS, K, GMAX, NDIF, MAX, NN, G

COMPLEX

A(32000), VZ(32000), X

REAL

FREQ(505), WK(534), AV(500)

INTEGER

IWK(100), N, IINJ, ILTO, IFLAG

FUNDAMENTAL CONSTANTS

H=1.05459
E=1.60219
C=4.803213
KB=1.38062
M=9.109136

DATA ON MATERIAL GAAS

WRITE(5,41)
41 FORMAT(10X,'MATERIAL DENSITY(GM.CM-3)')
READ(8,689)RHE
WRITE(5,42)
42 FORMAT(10X,'VELOCITY OF SOUND(10**5CM,S-1)')
READ(8,689)S
WRITE(5,43)
43 FORMAT(10X,'HIGH FREQUENCY DIELECTRIC CONSTANT')
READ(8,689)R1
WRITE(5,44)
44 FORMAT(10X,'LOW FREQUENCY DIELECTRIC CONSTANT')
READ(8,689)R2
WRITE(5,1)
1 FORMAT(10X,'OPTICAL PHONON FREQUENCY(10**13RAD.S-1)')
READ(8,689)WO
WRITE(5,2)
2 FORMAT(10X,'EQU. INTERVALLEY PHONON FREQ.')
READ(8,689)WE
WRITE(5,3)
3 FORMAT(10X,'NON.EQUIV. INTERVALLEY PHONON FREQ.')
READ(8,689)W
WRITE(5,4)
4 FORMAT(10X,'ACOUSTIC DEFORMATION POTENTAL(EV)')
READ(8,689)THA
WRITE(5,500)THA
500 FORMAT(10X,E10.4)
WRITE(5,1001)
1001 FORMAT(10X,'EQU. INTER. COUPLING CONST. L-L')
READ(8,689)THELL
WRITE(5,688)THELL
WRITE(5,1003)
1003 FORMAT(10X,'EQU. INTER. COUPLING CONST. X-X')
READ(8,689)THEXX
WRITE(5,688)THEXX
WRITE(5,1005)
WRITE(7,1005)
1005 FORMAT(10X,'NON. EQU. INTER. COUPLING G-L')
READ(8,689)THIGL
WRITE(5,688)THIGL
WRITE(7,688)THIGL
WRITE(5,1007)
1007 FORMAT(10X,'NON. EQU. INTER. COUPLING G-X')
READ(8,689)THIGX
WRITE(5,688)THIGX
WRITE(5,1009)
1009 FORMAT(10X,'NON. EQU. INTER. COUPLING L-X')
READ(8,689)THILX
WRITE(5,688)THILX
WRITE(5,7)
7 FORMAT(10X,'G-L VALLEY SEPARATION')
READ(8,689)D
WRITE(5,688)D
WRITE(5,1011)
1011 FORMAT(10X,'G-X VALLEY SEPARATION')
READ(8,689)D2
WRITE(5,688)D2
WRITE(5,8)
8 FORMAT(10X,'CENTRAL(G) VALLEY EFFECTIVE MASS')
READ(8,689)EM1
WRITE(5,688)EM1
WRITE(5,9)
9 FORMAT(10X,'L VALLEY EFF. MASS')
READ(8,689)EM2
WRITE(5,688)EM2
WRITE(5,1013)
1013 FORMAT(10X,'X VALLEY EFF. MASS')
READ(8,689)EM3
WRITE(5,688)EM3
688 FORMAT(10X,E10.4)
689 FORMAT(E10.4)
C===============================================
C FINAL DATA INPUT
C===============================================
46 WRITE(5,10)
10 FORMAT(10X,'TEMPERATURE(KELVIN)')
READ(8,531) T
531 FORMAT(E10.4)
WRITE(5,21)
21 FORMAT(10X,'MAXIMUM ENERGY(EV)')
READ(8,532) EMAX
532 FORMAT(E10.4)
535 WRITE(5,11)
11 FORMAT(10X,'NUMBER OF AVERAGES')
18 READ(8,533) NDIF
533 FORMAT(15)
534 IF(THI.NE.0.0) GO TO 750
535 IF(NDIF.LE.3000) GO TO 16
536 WRITE(5,710)
710 FORMAT(10X,'MAXIMUM COLLISIONS IN ONE VALLEY=3000')
750 IF(NDIF.LE.20000) GO TO 16
17 WRITE(5,17)
12 FORMAT(10X,'NUMBER OF ELECTRIC FIELDS')
16 READ(8,534) NF
13 FORMAT(I2)
14 DO 30 I=1,NF
15 WRITE(5,13) I
16 FORMAT(10X,'FIELD*',I2)
17 READ(8,535) F(I)
30 CONTINUE
22 WRITE(5,22)
23 FORMAT(10X,'DISTANCE FROM KZ AXIS OF DISTRIBUTION :1 TO 21')
24 READ(8,537) VR
25 WRITE(5,23)
26 FORMAT(10X,'VALLEY FOR DISTRIBUTION FUNCTION :1,2,3')
27 READ(8,536) VV
28 WRITE(5,12)
29 FORMAT(E12.4)
30 CONTINUE
31 WRITE(5,23)
32 FORMAT(10X,'VALLEY FOR DISTRIBUTION FUNCTION :1,2,3')
33 READ(8,536) VV
34 WRITE(5,12)
35 FORMAT(E12.4)
36 CONTINUE
37 C===============================================================
38 C CALCULATE PHONON FREQUENCIES AND OCCUPATION RATIOS
39 C===============================================================
40 HWO=H*WO/(E*100.0)
41 HWI=H*WI/(E*100.0)
42 HWE=H*WE/(E*100.0)
43 IF(WO.NE.0.0) GO TO 909
44 NO=0.0
45 GO TO 908
46 NO=1/(EXP((WO*76.385)/T)-1)
47 NI=1/(EXP((WI*76.385)/T)-1)
48 NE=1/(EXP((WE*76.385)/T)-1)
49 C===============================================================
50 C CONSTANTS FOR SCATTERING RATES
51 C===============================================================
52 C POLAR OPTICAL E/A
53 C1=1.0E+12*C2*SQRT(M)*WO*(1/R1-1/R2)*(NO+1)/(1.4142*H*SQRT(E))
54 C2=C1*NO/(NO+1)
55 C ACoustic (Both E/A)
56 C3=1.0E+10*(2*M)**1.5*KB*THA*THA*E*SQRT(E)/(4.0*3.142*RHE
57 C 1*S*H*H*H*H)
58 C EQUIVALENT INTERVALLEY
C

L-L E/A
C4=3.0E+14*M**1.5*THEL*THEL*E*E*(NE+1)*SQRT(E)
1/(1.4142*3.142*RHE*WE*H*H*H)
C5=C4*NE/(NE+1)
C

X-X E/A
C6=2.0E+14*M**1.5*THEXX*THEXX*E*E*(NE+1)*SQRT(E)
1/(1.4142*3.142*RHE*WE*H*H*H)
C7=C6*NE/(NE+1)

C

NONEQUIVALENT INTERVALLEY
G,L,X E/A
C8=1.0E+14*(EM1*M)**1.5*E*E*(NI+1)*SQRT(E)/(1.4142
1*3.142*RHE*WI*H*H*H)
C9=4.0E+14*(EM2*M)**1.5*E*E*(NI+1)*SQRT(E)/(1.4142
1*3.142*RHE*WI*H*H*H)
C10=3.0E+14*(EM3*M)**1.5*E*E*(NI+1)*SQRT(E)/(1.4142
1*3.142*RHE*WI*H*H*H)
C11=C8*NI/(NI+1)
C12=C9*NI/(NI+1)
C13=C10*NI/(NI+1)

C===============================================r=============r

DK(1)=1.0E+7*SQRT(2*EM1*M*EMAX*E)/(H*20.0)
DK(2)=1.0E+7*SQRT(2*EM2*M*EMAX*E)/(H*20.0)
DK(3)=1.0E+7*SQRT(2*EM3*M*EMAX*E)/(H*20.0)

C===============================================r=============r

KZI=-DK(W)*9.5
DO 805 LL=1,20
WRITE(5,807) KZI
807 FORMAT(E12.4)
KZI=KZI+DK(W)
805 CONTINUE

C

SET PARAMETERS FOR CENTRAL VALLEY, THEN CALCULATE THE
C TOTAL SCATTERING RATE FOR REAL PROCESSES (R) FOR A NUMBER
C OF ENERGIES UP TO THE MESH SIZE. STORE MAXIMUM VALUE OF R
C IN GAMMA(1) TO CALCULATE PSEUDO (SELF) SCATTERING RATE.
C TT=1 ENABLES PROGRAM TO RETURN TO LABEL 40

TT=1
EM=EM1
V=1
31 GAMMA(V)=0.0
EI=0.0
J=1
35 EI=EI+EMAX/20.0
GO TO 100
40 R=0.0
DO 50 I=1,18
R=R+L(I)
CONTINUE
IF(R.GT.GAMMA(V)) GAMMA(V)=R
J=J+1
IF(J.NE.21) GO TO 35
C===================================================================
C SET PARAMETERS FOR SATELLITE VALLEYS AND REPEAT PROCESS
C TO OBTAIN GAMMA(2) AND GAMMA(3)
C===================================================================
IF(V.EQ.3) GO TO 71
IF(V.EQ.2) GO TO 70
EM=EM2
V=2
GO TO 31
70 EM=EM3
V=3
GO TO 31
71 WRITE(5,75) GAMMA(1),GAMMA(2),GAMMA(3)
WRITE(7,75) GAMMA(1),GAMMA(2),GAMMA(3)
75 FORMAT(5X,'GAMMA(1)='E10.4,'GAMMA(2)='E10.4,'GAMMA(3)='E10.4)
WRITE(5,72) T,NDIF,EMAX
WRITE(7,72) T,NDIF,EMAX
72 FORMAT(10X,'TEMP='E10.4,5X,'NUM FLIGHT='I4,5X,'MAXENERGY='E10.4)
WRITE(5,600)
WRITE(7,600)
600 FORMAT('FIELD VAV IINJ ILTO N GMAX IDIF')
C===================================================================
C SET MESH REGISTERS TO ZERO AND PLACE ELECTRON AT
C STARTING POINT IN MESH.TT=0 FOR ITERATIVE PROCESS
C===================================================================
TT=0
J=1
TTOT=0.0
VAV=0.0
VAVG=0.0
V2AVG=0.0
DIF=0.0
V3AVG=0.0
V4AVG=0.0
DIF4=0.0
CHECK=0.0
TF=100E-12
FT=TF
DT=2.5E-14
IDIF=0
ETOT=0.0
KZTOT=0.0
TIM1=0.0
TIM2=0.0
TIM3=0.0
MAXE=0.0
MAX=0
N=0
NN=0
TIMEV=0.0
TIMEX=0.0
TIMXX=0.0
SR=0
SS=0
GMAX=0
LGTH=4.0E-4
WRITE(5,79) LGTH
WRITE(7,79) LGTH
79 FORMAT(2X,'DEVICE LENGTH= ',E10.4)
IINJ=0
ILT0=0
IFLAG=0
NPRINT=0

C===================================================================
C INJECT NEW ELECTRON AT Z=0 USING
C MODIFIED MAXWELLIAN DISTRIBUTION IN ENERGY
C===================================================================

80 V=1
   EM=EM1
   IF(IFLAG.EQ.1) ILT0=ILT0+1
   IFLAG=0
   IINJ=IINJ+1
   R=RANU(0.0,1.0)
   IF(R.EQ.0.0) R=1.0E-20
   EZ=8.63E-5*T*ALOG(1/R)
   KZF=(1.0E+7)*SQRT(ABS(2*EM*M*EZ*E))/H
   R=RANU(0.0,1.0)
   IF(R.EQ.0.0) R=1.0E-20
   ERHO=8.63E-5*T*ALOG(1/R)
   KRHO=(1.0E7)*SQRT(ABS(2*EM*M*ERHO*E))/H
   ZIN=0.0
   Z=0.0

C===================================================================
C CALL RANDOM NUMBER(N0T=0) AND CALCULATE TIME OF
C FLIGHT UNDER ELECTRIC FIELD AND NEW POSITION OF
C ELECTRON K SPACE
C===================================================================

90 R=RANU(0.0,1.0)
   IF(R.EQ.0.0) R=1.0E-20
   TIME=-ALOG(R)/GAMMA(V)
   KZI=KZF+(TIME*E*F(J)*1.0E+18)/H
   KT=SQRT(KRHO*KRHO+KZI*KZI)
   EI=H*H*KT*KT*1.0E-14/(E*2*EM*M)

C===================================================================
C CHECK FOR Rounding ERRORS LEADING TO NEGATIVE ENERGY VALUES.
C IF THIS OCCURS, PLACE ELECTRON AT STARTING POSITION.
C===================================================================

   IF(EI.GT.0.0) GO TO 96
   KRHO=0.0
   KZF=1.0E+6
   EM=EM1
   V=1
   GO TO 90
C IF ELECTRON LEAVES MESH PLACE IT ON EDGE OF MESH AND
C REGISTER OCCURRENCE IN COUNTER GMAX
C===============================================
96 IF(EI.GT.MAXE) MAXE=EI
   IF(EI.LE.EMAX) GO TO 95
   EI=EMAX
   KT=1.0E+7*SQRT(2*EM*M*EMAX*E)/H
   IF(KZI.GT.0.0) GO TO 94
   KZI=-SQRT(ABS(KT*KT-KRHO*KRHO))
   GO TO 95
94 KZI=SQRT(ABS(KT*KT-KRHO*KRHO))
C===============================================
C CHECK IF INITIAL VELOCITY AFTER COLLISION IS LESS THAN ZERO
C IF YES CHECK TO SEE IF ELECTRON POSITION GOES LESS THAN ZERO
C DURING THE FLIGHT
C===============================================
95 ACCEL=(E*F(J)/M*EM)**1.0E+19
VIN=1.15767*KZF/EM
   IF(VIN.GT.0.0) GO TO 82
C===============================================
C CALCULATE MINIMUM POSITION ZMIN
C===============================================
   TMIN=-VIN/ACCEL
   IF(TMIN.GT.TIME) GO TO 88
   ZMIN=ZIN+VIN*TMIN+.5*ACCEL*TMIN**2
   IF(ZMIN.GT.0.0) GO TO 82
   GO TO 89
88 Z=ZIN+VIN*TIME+.5*ACCEL*TIME**2
   IF(Z.GT.0.0) GO TO 82
89 IFLAG=1
   B=SQRT(VIN**2-2*ACCEL*ZIN)
   TIME=(-VIN+B)/ACCEL
   GO TO 83
C===============================================
C CHECK FOR Z > LGTH
C===============================================
82 Z=ZIN+VIN*TIME+.5*ACCEL*TIME**2
C WRITE(5,81)Z,V,IINJ,ILTO
C WRITE(7,81)Z,V,IINJ,ILTO
C1 FORMAT(5X,E10.4,5X,I5,1X,I5,1X,I5)
   IF(Z.LT.LGTH) GO TO 83
   IFLAG=2
   B=SQRT(VIN**2-2*ACCEL*(ZIN-LGTH))
   TIME=(-VIN-B)/ACCEL
C===============================================
C LOOP TO GENERATE VELOCITY TIME SERIES
C===============================================
C CHECK TO SEE IF FLIGHT LONG ENOUGH.
C IF NOT GO TO NEXT SCATTERING EVENT
C AFTER UPDATING TIMEX
C===============================================
83 ZIN=Z
IF(TIME.GT.0.0) GO TO 84
WRITE(5,85)
WRITE(7,85)

85 FORMAT(2X,'ERROR; NEGATIVE TIME GENERATED')
GO TO 1000

84 IF(V.EQ.1) TIM1=TIM1+TIME
IF(V.EQ.2) TIM2=TIM2+TIME
IF(V.EQ.3) TIM3=TIM3+TIME
TIMXX=TIMEX+TIME
IF(TIMXX.GT.DT) GO TO 97
TIMEX=TIMEX+TIME
IF(IFLAG.EQ.0) GO TO 100
GO TO 80

C==============================================
C ADVANCE TO NEXT DT AND CALCULATE
C==============================================

97 KZFV=KZF
TIMEV=DT-TIMEX
N=N+1
KZIV=KZFV+(TIMEV*E*F(J)*1.0E+18)/H
VZ(N)=1.15767*KZIV/EM
KZFV=KZIV
IF(N.EQ.4000) GO TO 473

C==============================================
C ADJUST TIME OF FLIGHT REMAINING AND CALC LOOP
C IF NN=0 UPDATE TIMEX AND GO SCATTER
C==============================================

TIME=TIME-(DT-TIMEX)
NN=TIME/DT
IF(NN.NE.O) GO TO 98
TIMEX=TIME
IF(IFLAG.EQ.0) GO TO 100
GO TO 80

98 DO 99 G=1,NN
N=N+1
TIMEV=DT
KZIV=KZFV+(TIMEV*E*F(J)*1.0E+18)/H
VZ(N)=1.15767*KZIV/EM
KZFV=KZIV
IF(N.EQ.4000) GO TO 473

99 CONTINUE
TIMEX=TIME-NN*DT
IF(IFLAG.EQ.0) GO TO 100
GO TO 80

C==============================================
C CALCULATE FINAL ENERGY VALUE FOR EACH SCATTERING PROCESS
C==============================================

C POLAR OPTICAL E/A
100 EF(1)=EI-HWO
EF(2)=EI+HWO
C ACOUSTICAL E/A
EF(3)=EI
EF(4)=EI
C EQUIVALENT INTERVALLEY E/A
EF(5) = EI - HWE
EF(6) = EI + HWE

C
  NON-EQUIVALENT INTERVALLEY
C
  G -> L E/A
EF(7) = EI - HWI - D
EF(8) = EI + HWI - D
C
  G -> X E/A
EF(9) = EI - HWI - D2
EF(10) = EI + HWI - D2
C
  L -> G E/A
EF(11) = EI - HWI + D
EF(12) = EI + HWI + D
C
  L -> X E/A
EF(13) = EI - HWI - (D2 - D)
EF(14) = EI + HWI - (D2 - D)
C
  X -> G E/A
EF(15) = EI - HWI + D2
EF(16) = EI + HWI + D2
C
  X -> L E/A
EF(17) = EI - HWI + D2 - D
EF(18) = EI + HWI + D2 - D

C
  SCATTERING RATES FOR REAL PROCESSES
C
  EMISSION OF OPTICAL PHONON
C
  IF(EF(1).GT.0.0) GO TO 110
L(1) = 0.0
  GO TO 120
110 L(1) = C1 * SQRT(EM) * ALOG(ABS((SQRT(EI) + SQRT(EF(1)))/(SQRT(EI) -
  1SQRT(EF(1)))))/SQRT(EI)
C
  ABSORPTION OF OPTICAL PHONON
C
  120 IF(EF(2).GT.0.0) GO TO 125
L(2) = 0.0
  GO TO 130
125 L(2) = C2 * SQRT(EM) * ALOG(ABS((SQRT(EI) + SQRT(EF(2)))/(SQRT(EI) -
  1SQRT(EF(2)))))/SQRT(EI)
C
  EMISSION OF ACOUSTIC PHONON
C
  130 IF(EF(3).GT.0.0) GO TO 135
L(3) = 0.0
  GO TO 140
135 L(3) = C3 * EM**1.5 * SQRT(EF(3))
C
  ABSORPTION OF ACOUSTIC PHONON
C
  140 IF(EF(4).GT.0.0) GO TO 145
L(4) = 0.0
  GO TO 150
145 L(4) = L(3)
C
C
C
C
C
C
C
C
C EQUIVALENT INTERVALLEY L OR X
C EMISSION OF PHONON
C===================================================================
150 IF(EF(5).LT.0.0) GO TO 152
   IF(V.EQ.1) GO TO 152
   IF(V.EQ.3) GO TO 151
C L VALLEY
   L(5)=C4*EM**1.5*SQRT(EF(5))
   GO TO 160
C X VALLEY
151 L(5)=C6*EM**1.5*SQRT(EF(5))
   GO TO 160
152 L(5)=0.0
C===================================================================
C EQUIVALENT INTERVALLEY L OR X
C ABSORPTION OF PHONON
C===================================================================
160 IF(EF(6).LT.0.0) GO TO 162
   IF(V.EQ.1) GO TO 162
   IF(V.EQ.3) GO TO 161
C L VALLEY
   L(6)=C5*EM**1.5*SQRT(EF(6))
   GO TO 170
C X VALLEY
161 L(6)=C7*EM**1.5*SQRT(EF(6))
   GO TO 170
162 L(6)=0.0
C===================================================================
C NONEQUIVALENT INTERVALLEY
C===================================================================
C   G -> L EMISSION OF PHONON
170 IF(EF(7).LT.0.0) GO TO 171
   IF(V.EQ.2) GO TO 171
   IF(V.EQ.3) GO TO 171
   L(7)=C9*SQRT(EF(7))*THIGL*THIGL
   GO TO 180
171 L(7)=0.0
C   G -> L ABSORPTION OF PHONON
180 IF(EF(8).LT.0.0) GO TO 181
   IF(V.EQ.2) GO TO 181
   IF(V.EQ.3) GO TO 181
   L(8)=C12*SQRT(EF(8))*THIGL*THIGL
   GO TO 190
181 L(8)=0.0
C   G -> X EMISSION OF PHONON
190 IF(EF(9).LT.0.0) GO TO 191
   IF(V.EQ.2) GO TO 191
   IF(V.EQ.3) GO TO 191
   L(9)=C10*SQRT(EF(9))*THIGX*THIGX
   GO TO 200
191 L(9)=0.0
C
C G -> X ABSORPTION OF PHONON 200 IF(EF(10).LT.0.0) GO TO 201 IF(V.EQ.2) GO TO 201 IF(V.EQ.3) GO TO 201 L(10)=C13*SQRT(EF(10))*THIGX*THIGX GO TO 210 201 L(10)=0.0 C C L -> G EMISSION OF PHONON 210 IF(EF(11).LT.0.0) GO TO 211 IF(V.EQ.1) GO TO 211 IF(V.EQ.3) GO TO 211 L(11)=C8*SQRT(EF(11))*THIGL*THIGL GO TO 220 211 L(11)=0.0 C C L -> G ABSORPTION OF PHONON 220 IF(EF(12).LT.0.0) GO TO 221 IF(V.EQ.1) GO TO 221 IF(V.EQ.3) GO TO 221 L(12)=C11*SQRT(EF(12))*THIGL*THIGL GO TO 225 221 L(12)=0.0 C C L -> X EMISSION OF PHONON 225 IF(EF(13).LT.0.0) GO TO 226 IF(V.EQ.1) GO TO 226 IF(V.EQ.3) GO TO 226 L(13)=C10*SQRT(EF(13))*THILX*THILX GO TO 230 226 L(13)=0.0 C C L -> X ABSORPTION OF PHONON 230 IF(EF(14).LT.0.0) GO TO 231 IF(V.EQ.1) GO TO 231 IF(V.EQ.3) GO TO 231 L(14)=C13*SQRT(EF(14))*THILX*THILX GO TO 235 231 L(14)=0.0 C C X -> G EMISSION OF PHONON 235 IF(EF(15).LT.0.0) GO TO 236 IF(V.EQ.1) GO TO 236 IF(V.EQ.2) GO TO 236 L(15)=C8*SQRT(EF(15))*THIGX*THIGX GO TO 240 236 L(15)=0.0 C C X -> G ABSORPTION OF PHONON 240 IF(EF(16).LT.0.0) GO TO 241 IF(V.EQ.1) GO TO 241 IF(V.EQ.2) GO TO 241 L(16)=C11*SQRT(EF(16))*THIGX*THIGX GO TO 245
L(16)=0.0

X -> L  EMISSION OF PHONON

IF(EF(17).LT.0.0) GO TO 246
IF(V.EQ.1) GO TO 246
IF(V.EQ.2) GO TO 246
L(17)=C9*SQRT(EF(17))*THILX*THILX
GO TO 250

L(17)=0.0

X -> L  ABSORPTION OF PHONON

IF(EF(18).LT.0.0) GO TO 251
IF(V.EQ.1) GO TO 251
IF(V.EQ.2) GO TO 251
L(18)=C12*SQRT(EF(18))*THILX*THILX
GO TO 270

L(18)=0.0

IF(TT.EQ.1) GO TO 40

C===============================================
C  CALCULATE SUM OF REAL PROCESS SCATTERING RATES
C===============================================

SCATT(1)=L(1)/GAMMA(V)
DO 290 K=2,18
SCATT(K)=SCATT(K-1)+L(K)/GAMMA(V)
290 CONTINUE

IF(1.0-SCATT(18).LT.0.0) THEN
WRITE(5,295)
WRITE(7,295)
FORMAT('NEGATIVE SELFSCATTERING RATE')
MAX=MAX+1
IF(MAX.EQ.100) GO TO 1000
END IF

C===============================================
C  CALL RANDOM NUMBER.SELECT SCATTERING CHANNEL
C===============================================

R=RANU(0.0,1.0)
IF(R.LT.SCATT(1)) GO TO 300
IF(R.LT.SCATT(2)) GO TO 310
IF(R.LT.SCATT(3)) GO TO 320
IF(R.LT.SCATT(4)) GO TO 330
IF(R.LT.SCATT(5)) GO TO 340
IF(R.LT.SCATT(6)) GO TO 350
IF(R.LT.SCATT(7)) GO TO 360
IF(R.LT.SCATT(8)) GO TO 370
IF(R.LT.SCATT(9)) GO TO 380
IF(R.LT.SCATT(10)) GO TO 390
IF(R.LT.SCATT(11)) GO TO 391
IF(R.LT.SCATT(12)) GO TO 392
IF(R.LT.SCATT(13)) GO TO 393
IF(R.LT.SCATT(14)) GO TO 394
IF(R.LT.SCATT(15)) GO TO 395
IF(R.LT.SCATT(16)) GO TO 396
IF(R.LT.SCATT(17)) GO TO 397
IF(R.LT.SCATT(18)) GO TO 398
GO TO 400

C=================================================================================================================================
C SET ENERGY AFTER SCATTERING PROCESS
C=================================================================================================================================

300  EFIN=EF(1)
       GO TO 420
310  EFIN=EF(2)
       GO TO 420
320  EFIN=EF(3)
       GO TO 420
330  EFIN=EF(4)
       GO TO 420
340  EFIN=EF(5)
       GO TO 420
350  EFIN=EF(6)
       GO TO 420
360  EFIN=EF(7)
       GO TO 431
370  EFIN=EF(8)
       GO TO 431
380  EFIN=EF(9)
       GO TO 432
390  EFIN=EF(10)
       GO TO 432
391  EFIN=EF(11)
       GO TO 430
392  EFIN=EF(12)
       GO TO 430
393  EFIN=EF(13)
       GO TO 432
394  EFIN=EF(14)
       GO TO 432
395  EFIN=EF(15)
       GO TO 430
396  EFIN=EF(16)
       GO TO 430
397  EFIN=EF(17)
       GO TO 431
398  EFIN=EF(18)
       GO TO 431
400  EFIN=EI
       GO TO 450

C=================================================================================================================================
C REGISTER REAL COLLISION.CALCULATE K SPACE POSITION AFTER
C ACOUSTIC,INTERVALLEY OR EQUIVALENT INTERVALLEY PHONON SCATTERING
C=================================================================================================================================

410  SR=SR+1
       R=RANU(0.0,1.0)
       KT=1.0E+7*SQRT(2*EM*M*EFIN*E)/H
       KZF=KT*(1-2*R)
       KRHO=KT*SQRT(4*R*(1-R))
       GO TO 460

C=================================================================================================================================
C REGISTER REAL COLLISION, CALCULATE K SPACE POSITION AFTER
C OPTICAL PHONON SCATTERING
C===============================================================
  420  SR=SR+1
       R=RANU(0.0,1.0)
       U=RANU(0.0,1.0)
       PHI=2*3.142*R
       EX=2*SQRT(EFIN*EI)/((SQRT(EI)-SQRT(EFIN))^2)
       BETA=((1+EX)-(1+2*EX)^2)/EX
       RHO=(BETA*KZI/HT-SQRT(ABS(1-BETA*BETA))*KRHO/HT*COS(PHI))
       KT=1.0E+7*SQRT(2*EM*M*EFIN*E)/H
       KZF=KT*RHO
       KRHO=KT*SQRT(ABS(1-RHO*RHO))
       GO TO 460
C===============================================================
C CHANGE VALLEY PARAMETERS FOR INTERVALLEY PROCESSES.
C===============================================================
  430  V=1
       EM=EM1
       GO TO 410
  431  V=2
       EM=EM2
       GO TO 410
  432  V=3
       EM=EM3
       GO TO 410
C===============================================================
C REGISTER SELF SCATTERING PROCESS. K SPACE POSITION UNCHANGED
C===============================================================
  450  SS=SS+1
       KZF=KZI
       KT=SQRT(KZF*KZF+KRHO*KRHO)
       EFIN=H*H*KT*KT*1.0E-14/(E^2*EM^M)
C===============================================================
C CHECK IF ELECTRON IS SCATTERED OUT OF MESH. IF SO, REGISTER
C PROCESS ON COUNTER GMAX, AND PLACE ELECTRON ON EDGE OF MESH
C LABEL 90 REPEATS ITERATIVE PROCESS STARTING WITH FREE
C ELECTRON FLIGHT UNDER ELECTRIC FIELD.
C===============================================================
  460  IF(EFIN.LE.EMAX) GO TO 90
       GMAX=GMAX+1
       KT=1.0E+7*SQRT(2*EM*M*EMAX*E)/H
       IF(KRHO.GT.KT) KRHO=KT
       KZF=SQRT(ABS(KT*KT-KRHO*KRHO))
       GO TO 90
C===============================================================
C FINAL CALCULATIONS OF TIME SERIES AFTER N POINTS HAVE
C BEEN GENERATED.
C===============================================================
  473  IDIF=IDIF+1
       NPRINT=NPRINT+1
       VA=0.0
       DO 481 G=1,N
       VA=VA+VZ(G)
       GO TO 481
CONTINUE

VA=VA/N
VAV=(VAV*(IDIF-1)+VA)/IDIF

C=================================================================
C REMOVE AVERAGE VELOCITY, PUT IN VECTOR A
C=================================================================

DO 482 G=1,N
A(G)=VZ(G)-VA

482 CONTINUE

WRITE(5,480)F(J),VAV,INJ,ILTO,N,GMAX,IDIF
WRITE(7,480)F(J),VAV,INJ,ILTO,N,GMAX,IDIF
480 FORMAT(2(E9.3,1X),1X,I6,1X,I5,1X,I5,1X,I5,1X,I5)
IF(IDIF.LT.NDIF) GO TO 490
WRITE(5,492)
WRITE(7,492)

492 FORMAT(1X,'POPULATION GAM L X')
TOTVT=TIM1+TIM2+TIM3
TIM1=TIM1/TOTVT
TIM2=TIM2/TOTVT
TIM3=TIM3/TOTVT
WRITE(5,493)TIM1,TIM2,TIM3
WRITE(7,493)TIM1,TIM2,TIM3
493 FORMAT(10X,3(E9.3,1X))

CALL FFTRC TO CALCULATE FFT OF TIME SERIES

CALL FFTRC (A,N,X,IWK,WK)

WRITE(5,800)
WRITE(7,800)
800 FORMAT(10X,'FREQUENCY',5X,'FFT DIFFUSION CM2/SEC')

DO 830 G=1,400
FREQ(G)=(G-1)/100.0E-12
A(G)=X(G)*CONJG(X(G))*3.127E-18
AV(G)=(AV(G)*(IDIF-1)+A(G))/IDIF
WRITE(5,810) FREQ(G),AV(G)
IF(IDIF.LT.NDIF) GO TO 815
WRITE(7,810) FREQ(G),AV(G)
815 CONTINUE
810 FORMAT(5X,E10.4,10X,E10.4)
830 CONTINUE

N=0
MPRINT=0
IF(IDIF.LT.NDIF) GO TO 80
IDIF=0
J=J+1
IF(J .NE. NF+1) GO TO 80
1000 STOP
END
REFERENCES

BIографICAL SKETCH

Christopher Francis Whiteside was born in Coral Gables, Florida, on August 2, 1959. In August of 1982 he received the degree of Bachelor of Science in Electrical Engineering, with honors, from the University of Florida. He received the Master of Engineering degree from the University of Florida in December of 1983.

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May 1987  

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