ELECTRON TRANSPORT PHENOMENA IN A NON-DEGENERATE SEMICONDUCTOR AT HIGH FIELDS

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ABSTRACT

The effects of a third valley, transverse magnetic field, traps, and impact ionisation on the steady state current-voltage characteristics of a non-degenerate semiconductor having the appropiate band structure for the occurrence of Gunn instabilities have been analysed. For n-GaAs, the presence of a third valley does not change the threshold field, while the application of a transverse magnetic field raises the threshold field slightly. The presence of traps has a significant effect on the steady state current-voltage characteristics even though the trapping rates may be very much smaller than the intervalley transfer rates. Impact ionisation does not totally preclude the occurrence of Gunn instabilities unless its rate is very much greater than the intervalley transfer rates. A very strong field dependence of the impact ionisation rate is also a hindrance.

The threshold field for the occurrence of negative differential resistance due to field-enhanced carrier-trapping has been calculated. The theoretical results for n-GaAs are in good agreement with presently available experimental results.

It is also shown that negative differential resistance can be produced in a two-valley semiconductor by Joule heating.

Coherent oscillations were observed in freshly prepared n-GaAs samples of 1 cm. in length. The sample properties were degraded after the samples had been stored in a dry atmosphere for a few months, and this is attributed to the surface effect.

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LIST OF MOST USED SYMBOLS

e	electronic charge
E	applied electric field
$\mathcal{E}$	carrier energy
$f(\vec{p})$	carrier distribution function
$\left(\frac{\partial f}{\partial t}\right)_{e-e}$	carrier-carrier scattering
$\left(\frac{\partial f}{\partial t}\right)_{scatt}$	carrier-phonon scattering
f_{eq}	equilibrium carrier distribution function
f_o	first term in Legendre series expansion of f
f_1	carrier distribution function for the lower valley
f_2	carrier distribution function for the upper valley
f_{10}	first term in Legendre series expansion of f_1
f_{20}	first term in Legendre series expansion of f_2
$\hbar$	Planck's constant divided by 2π
H'	electron-phonon interaction Hamiltonian
$\vec{J}$	current density
k_B	Boltzmann's constant
$\vec{k}$	carrier wave vector
m^*, m	carrier effective mass
m_1^*	carrier effective mass in the lower valley
m_2^*	carrier effective mass in the upper valley
N_q	equilibrium phonon distribution
n	carrier concentration
n_1	carrier concentration in the lower valley

n_2	carrier concentration in the upper valley
$\vec{p}$	carrier momentum
$\vec{p}_o$	momentum displacement induced by applied field
p_E	carrier momentum in the direction of the field
$\vec{q}$	phonon momentum
T_o, T	lattice temperature
T_e	carrier temperature
T_1	carrier temperature in the lower valley
T_2	carrier temperature in the upper valley
$\vec{v}$	carrier velocity
v	carrier drift velocity
ω_q	phonon angular frequency
ω_e	angular frequency of phonons in polar scattering
τ	momentum relaxation time
μ_1	carrier mobility in the lower valley
μ_2	carrier mobility in the upper valley
τ_{po}	momentum relaxation time due to polar scattering
τ_{iv}	momentum relaxation time due to intervalley scattering
$\tau^{(i)}$	total momentum relaxation time in the i^{th} valley
$\frac{1}{\tau_{12}}$	rate of electron transfer from lower valley to upper valley per electron in the lower valley
$\frac{1}{\tau_{21}}$	rate of electron transfer from upper valley to lower valley per electron in the upper valley

CHAPTER 1

INTRODUCTION

Since 1950, considerable attention had been directed to the electronic transport phenomena in semiconductors under high electric fields; and for electron device applications, there had been an arduous search for materials in which negative differential resistances (NDR) could be easily produced. The many endeavours in these two directions were climaxed by the discovery of the Gunn Effect (Gunn, 1964) and the subsequent experimental and theoretical works on this phenonmenon. In view of the conclusive evidences provided by the experiments of Hutson et al (1965) and Allen et al (1965), it is now widely believed that the Gunn Effect is due to the field-enhanced transfer of electrons from a high mobility and low energy conduction subband to low mobility and high energy conduction subband. Such an intervalley transfer process had actually been conceived prior to the discovery of the Gunn Effect (Ridley and Watkins, 1961; Hilsum, 1962). Surveying the published literature on the NDR resulting from this field-enhanced intervalley transfer process, (almost all the published works are on n-GaAs) it is found that because of the various approximations used in the theoretical models, there are quantitative discrepancies between theoretical and experimental results. Furthermore, there is disagreement among the experimental results (Conwell and Vassell, 1968). This state of art suggests that not only the theoretical models have to be improved, the significance of physical factors which so far have not been considered or have been considered to be neglegible must be examined or re-examined. The main purpose of the investigation being reported in this thesis is to examine the factors that affect the Gunn instabilities, and to study the conditions for their occurrence more thoroughly.

Since the intervalley process is essentially a high field transport phenonmenon, a review of the analytic approaches to such phenonmena is given in Chapter II. This is followed by a discussion of the possible mechanisms of NDR in a two-valley semiconductor and the space-charge instabilities associated with NDR in Chapter III. The significance of several physical factors which can modify the NDR due to intervalley transfer is discussed in Chapters IV, V and VI. The effects of a transverse magnetic field and a third conduction subband are considered in Chapter IV; the effect of traps is considered in Chapter V; and the effect of electron-hole generation is considered in Chapter VI. A calculation of the NDR due to field-enhanced carrier-trapping in n-GaAs is also given in Chapter V. Chapter VII explores the possibility of producing a NDR by Joule heating. Finally, Chapter VIII reports some new experimental results on the Gunn Effect in long n-GaAs samples.

CHAPTER II

HIGH FIELD TRANSPORT IN NON-DEGENERATE SEMICONDUCTORS

With the carrier distribution function f appropriately normalised, the current density $\vec{J}$ in a semiconductor subjected to an applied field can be calculated by

$$\vec{J} = \int e\vec{v}f d^3p \qquad (2.1)$$

where e is the electronic charge, $\vec{v}$ the velocity of the carrier and $\vec{p}$ the momentum of the carrier. The steady state distribution function is governed by the Boltzmann Transport Equation:

$$0 = \vec{E}.\frac{\partial f}{\partial \vec{p}} + \vec{v}.\frac{\partial f}{\partial \vec{r}} + \left(\frac{\partial f}{\partial t}\right)_{e-e} + \left(\frac{\partial f}{\partial t}\right)_{scatt} \qquad (2.2)$$

where the terms on the right have the following meanings:

$\vec{E}.\frac{\partial f}{\partial \vec{p}}$ -- the effect due to external field $\vec{E}$

$\vec{v}.\frac{\partial f}{\partial \vec{r}}$ -- the effect due to diffusion

$\left(\frac{\partial f}{\partial t}\right)_{e-e}$ -- the effect due to carrier-carrier scattering

$\left(\frac{\partial f}{\partial t}\right)_{scatt}$ -- the effect due to other carrier-scattering mechanisms

While the Boltzmann equation is definitely not a vigorous equation (Kadonoff, 1966), it is nevertheless adequate to account quantitatively for the transport properties in a non-degenerate semiconductor whose carrier concentration is less than about 10^{18} cm^{-3}.

On the assumption that there is no doping gradient and temperature gradient in the semiconductor under consideration, and that there is no external magnetic field present, the Boltzmann equation then becomes:

$$0 = e\vec{E}.\frac{\partial f}{\partial \vec{p}} + \left(\frac{\partial f}{\partial t}\right)_{e-e} + \left(\frac{\partial f}{\partial t}\right)_{scatt} \qquad (2.3)$$

where $\vec{E}$ is the applied electric field. Formally, the solution of this equation can be expanded in terms of the Legendre polynomials P_n:

$$f(\vec{p},\vec{E}) = \sum_{n=0}^{\infty} f_n(\mathcal{E},\vec{E})\; P_n(\cos\theta) \qquad (2.4)$$

where $\mathcal{E}$ is the carrier energy and θ the angle between $\vec{p}$ and $\vec{E}$. f_n are functions to be determined by the Boltzmann equation. Substituting Eqn. (2.4) into Eqn. (2.3), an infinite series of coupled equations in f_n , which is not even numerically tractable, is obtained. Approximations which introduce cut-off in the series must therefore be used.

In the absence of applied fields, diffusion effects and carrier scattering except carrier-carrier scattering, the steady state distribution function is determined by:

$$\left(\frac{\partial f}{\partial t}\right)_{e-e} = 0 \qquad (2.5)$$

The solution of this equation for a non-degenerate semiconductor, by virtue of the fact that carrier-carrier scattering is elastic, is the Maxwell-Boltzmann function:

$$f_{eq} = C \exp\left(\frac{-\mathcal{E}}{k_B T}\right) \tag{2.6}$$

where C is a normalisation constant, k_B the Boltzmann's constant, and T the temperature. In the presence of an applied field and carrier scatterings other than carrier-carrier scattering, f will depart from f_{eq}. An applied electric field forces the carriers to drift preferably in the direction of the field and increases the average energy of the carriers. The carrier scatterings, on the other hand, tend to oppose the carrier 'streaming' effect produced by the applied field and thus act as processes causing the momentum and energy losses, which are necessary for the carriers to achieve steady state under an applied field. The scattering processes contributing to $\left(\frac{\partial f}{\partial t}\right)_{scatt}$ include the scattering by phonons and the scattering by impurities, the scattering by other crystal imperfections such as dislocations being normally less important. Explicitly, $\left(\frac{\partial f(\vec{p})}{\partial t}\right)_{scatt}$ is the algebraic sum of the rate of change of f due to carriers being scattered into the state with momentum $\vec{p}$, denoted by A, and the rate of change of f due to carriers being scattered from the state with momentum $\vec{p}$, denoted by B :

$$\left(\frac{\partial f(\vec{p})}{\partial t}\right)_{scatt} = A - B \tag{2.7}$$

On the assumption that the first order perturbation approximation is valid, that the phonon distribution remains undisturbed, and that the probability factor $1 - f$ can be neglected, A and B for the scattering by phonons have the forms :

$$A = \frac{2\pi}{\hbar}\sum_{\vec{q}}\left|\langle\vec{p},\, N_{\vec{q}} + 1\,|H'|\,\vec{p} + \vec{q},\, N_{\vec{q}}\rangle\right|^2$$
$$\delta(\varepsilon_{\vec{p}} - \varepsilon_{\vec{p}+\vec{q}} + \hbar w_{\vec{q}})\ f(\vec{p} + \vec{q})$$
$$+ \frac{2\pi}{\hbar}\sum_{\vec{q}}\left|\langle\vec{p},\, N_{\vec{q}} - 1\,|H'|\,\vec{p} - \vec{q},\, N_{\vec{q}}\rangle\right|^2$$
$$\delta(\varepsilon_{\vec{p}} - \varepsilon_{\vec{p}-\vec{q}} - \hbar w_{\vec{q}})\ f(\vec{p} - \vec{q})$$
$$B = \frac{2\pi}{\hbar}\sum_{\vec{q}}\left|\langle\vec{p} + \vec{q},\, N_{\vec{q}} - 1\,|H'|\,\vec{p},\, N_{\vec{q}}\rangle\right|^2$$
$$\delta(\varepsilon_{\vec{p}+\vec{q}} - \varepsilon_{\vec{p}} - \hbar w_{\vec{q}})\ f(\vec{p})$$
$$+ \frac{2\pi}{\hbar}\sum_{\vec{q}}\left|\langle\vec{p} - \vec{q},\, N_{\vec{q}} + 1\,|H'|\,\vec{p},\, N_{\vec{q}}\rangle\right|^2$$
$$\delta(\varepsilon_{\vec{p}-\vec{q}} - \varepsilon_{\vec{p}} + \hbar w_{\vec{q}})\ f(\vec{p}) \qquad (2.8)$$

where $\hbar$ = Planck's constant divided by 2π

$\vec{q}$ = momentum of phonon

$w_{\vec{q}}$ = angular frequency of phonon

$N_{\vec{q}}$ = phonon equilibrium distribution

= $(\exp\frac{\hbar w_{\vec{q}}}{k_B T_o} - 1)^{-1}$, and T_o is the lattice temperature

H' = electron-phonon interaction Hamiltonian

As far as the system of carriers is concerned, all scattering processes contributing to $(\frac{\partial f}{\partial t})_{scatt}$ are inelastic. The effect of $(\frac{\partial f}{\partial t})_{scatt}$ will be more drastic the more inelastic and anisotropic these processes are.

It is obvious that when $(\frac{\partial f}{\partial t})_{e-e}$ predominates over $e\vec{E}.\frac{\partial f}{\partial \vec{p}}$ and $(\frac{\partial f}{\partial t})_{scatt}$, the solution f of Eqn. (2.3) will depart from f_{eq} only slightly. The same is true if $(\frac{\partial f}{\partial t})_{scatt}$ is more important than $(\frac{\partial f}{\partial t})_{e-e}$ and the relevant scattering processes are nearly elastic and isotropic, and the applied field strength is small enough so that the carrier 'streaming' remains small and the average carrier energy is not appreciably increased. Under any other circumstances, the departure of f from f_{eq} will be large. It can therefore be concluded that the selection of approximations used to solve Eqn. (2.3), or equivalently, the cut-off procedure introduced to the series given by Eqn. (2.4),must be considered in the light of the following points:

(i) Which is more important, $(\frac{\partial f}{\partial t})_{e-e}$ or $(\frac{\partial f}{\partial t})_{scatt}$? If $(\frac{\partial f}{\partial t})_{scatt}$ is more important, are the scattering processes concerned highly inelastic or anisotropic?

(ii) Is the range of applied fields sufficiently large to produce a large carrier 'streaming' or a considerable increase in the average carrier random energy?

2.1 With dominant carrier-carrier scattering

The Boltzmann H Theorem states that the dominance of carrier-carrier scattering will enforce a 'displaced' Maxwellian carrier distribution function which is given by

$$f_D = C_D \exp\frac{-(\vec{p} - \vec{p}_o)^2}{2mk_BT_e} \tag{2.9}$$

where C_D is the normalisation constant, m the carrier effective mass, $\vec{p}_o$ the momentum displacement induced by the applied field, and T_e is the carrier temperature which is, in general, different from the lattice temperature to allow for the change of average carrier random energy with the field. $\vec{p}_o$ and T_e are determined by the momentum and energy conservation conditions:

$$\int \left[e\vec{E}.\frac{\partial f}{\partial \vec{p}} + \left(\frac{\partial f}{\partial t}\right)_{scatt} \right] \vec{p}\, d^3p = 0 \tag{2.10}$$

$$\int \left[e\vec{E}.\frac{\partial f}{\partial \vec{p}} + \left(\frac{\partial f}{\partial t}\right)_{scatt} \right] \mathcal{E}\, d^3p = 0 \tag{2.11}$$

Carrier-carrier scattering, being elastic, does not contribute to the integrals. Thus the current density, as given in Eqn. (2.1), is

$$\vec{J} = ne\vec{p}_o/m \tag{2.12}$$

where n is the carrier concentration.

It has been pointed out by Paranjape et al (Paranjape &

Ambrose, 1964; Paranjape & De Alba, 1965) that, when the dominant scattering process contributing to $(\frac{\partial f}{\partial t})_{scatt}$ is the scattering by optical phonons and at fairly low temperatures, T_e can drop below T_o at low fields before increasing to a value greater than T_o at higher fields. It is safe to assume, however, that at room temperatures (about 300^oK) the carrier distribution function at low-fields can be approximated by an expansion of f_D to the first order in p_e. By setting $T_e = T_o$, Eqn.(29) then becomes

$$f_D = C_D \exp(\frac{-p^2}{2mk_BT_o})\left[1 + \frac{\vec{p}\cdot\vec{p}_o}{mk_BT_o}\right] \qquad (2.13)$$

In spite of the fact that the 'displaced' Maxwellian formulation [Eqn. (2.9)] was first introduced to account for breakdown phenomena in solids (Fröhlich & Paranjape, 1955), its success in this respect is still controversial. Nevertheless, it has been widely accepted as the basis for electron transport theories in semiconductors at pre-breakdown field strengths and under strong carrier-carrier scattering condition.

2.2 With non-dominant carrier-carrier scattering and small carrier 'streaming'

In accordance with the discussion given at the beginning of this Chapter, the following cases are considered:

(i) Nearly elastic and isotropic scattering at low fields

Under these conditions the carrier distribution function departs only very slightly from f_{eq}. Thus the solution of Eqn. (2.3) can be well approximated by the first two terms in series given by Eqn. (2.4), with $f_o = f_{eq}$ and $T = T_o$. The carrier distribution at low fields is therefore

$$f_L \simeq f_{eq} + p_E g \tag{2.14}$$

where p_E is the momentum in the direction of field E and g is a function of carrier energy. Substitution of Eqn. (2.14) into Eqn. (2.3) gives

$$e\vec{E}.\frac{\partial f_{eq}}{\partial \vec{p}} + \left(\frac{\partial (p_E g)}{\partial t}\right)_{scatt} = 0 \tag{2.15}$$

In this equation the term $e\vec{E}.\frac{\partial}{\partial p}(p_E g)$, which is of second order in E, has been dropped. Eqn. (2.15) is called the linearised Boltzmann equation. With the carrier distribution function in the form of Eqn. (2.14), $\left(\frac{\partial (p_E g)}{\partial t}\right)_{scatt}$ can be further simplified by the relaxation time approximation (Appendix I) as

$$\left(\frac{\partial (p_E g)}{\partial t}\right)_{scatt} = -\frac{p_E g}{\tau} \tag{2.16}$$

where τ is the momentum relaxation time defined by

$$\frac{1}{\tau} = \int (1 - \cos\theta')\, P(\theta')\, p^2 \sin\theta'\, d\theta'\, d\phi' \tag{2.17}$$

for elastic scattering, and

$$\frac{1}{\tau} = \int P(\vec{p},\vec{p}')\ d^3p' \tag{2.18}$$

for isotropic scattering. Combination of Eqns. (2.5) and (2.6) gives

$$p_E g = eE \frac{p_E}{mk_BT_o} \tau\ f_{eq} \tag{2.19}$$

and the current density $\vec{J}$,

$$\vec{J} = \frac{4ne^2}{3\sqrt{\pi}m} \frac{1}{(k_BT_o)^{5/2}} \int_0^\infty \exp\left(\frac{-\varepsilon}{k_BT_o}\right)\tau\varepsilon^{3/2} d\varepsilon . \vec{E} \tag{2.20}$$

in which the following conditions have been used:

for the normalisation,

$$\int f_{eq} d^3p = n \tag{2.21}$$

and for the energy,

$$\frac{p_E^2}{2m} = \frac{1}{3}\frac{p^2}{2m} \tag{2.22}$$

(ii) Nearly elastic and isotropic scattering at intermediate fields

Intermediate fields are referred to the fields which are not high enough to produce large carrier 'streaming', but enough to increase significantly the average carrier energy. Under such conditions, the carrier distribution function can still be approximated by the first two terms of the series given in Eqn. (2.4)

$$f = f_o + p_E g \qquad (2.23)$$

But in this case f_o will be quite different from f_{eq}. In general, f_o and g have to be determined by the following equations, obtained by substituting Eqn. (2.23) into Eqn. (2.3), and using the relaxation time approximation:

$$\left.\begin{aligned} e\vec{E}.\frac{\vec{p}}{m}\, p_E \frac{dg}{d\varepsilon} + \left(\frac{\partial f_o}{\partial t}\right)_{scatt} &= 0 \\ e\vec{E}.\frac{\vec{p}}{m}\frac{df_o}{d\varepsilon} - \frac{p_E g}{\tau} &= 0 \end{aligned}\right\} \qquad (2.24)$$

The current density in this case is given by

$$\vec{J} = \frac{\frac{2}{3}\, ne \int_0^\infty g\, \varepsilon^{3/2} d\varepsilon}{\int_0^\infty f_o \varepsilon^{\frac{1}{2}} d\varepsilon} \qquad (2.25)$$

Without further approximation, it is not possible to obtain the solution of Eqn. (2.24) in analytical forms. One approximation that had been proposed is expanding f_o to terms of order E^2 (Yamashita, 1960)

$$f_o \simeq A_o\left[1 + E^2 \xi(\varepsilon)\right] \exp\left(\frac{-\varepsilon}{k_B T_o}\right) \qquad (2.26)$$

where A_o is the normalisation constant, and $\xi(\varepsilon)$ is a function independent of E.

(iii) Predominantly inelastic or anisotropic scattering

As pointed out earlier in this Chapter, the effect of predominantly inelastic or anisotropic scattering is rather drastic. In general, the approximation of keeping just two terms in the series given by Eqn. (2.4) is not justified.

Without considering its validity, the electron mobility due to polar optical scattering, which is inelastic and anisotropic, had been calculated by Howarth and Sondheimer (1953) and Ehrenreich (1957, 1959) by assuming the approximation given by Eqn. (2.14). Because a relaxation time cannot be defined for an inelastic and anisotropic scattering process, they resorted to the variational method (Ziman, 1962). The variational method will not be described further in this thesis. Suffice it to say that this method can only be applied to the linearised Boltzmann equation and therefore to cases where the steady state carrier distribution function departs only slightly from f_{eq}.

2.3 With equally important carrier-carrier scattering and other carrier scattering processes

Theoretically, the distribution function for the case where $(\frac{\partial f}{\partial t})_{e-e}$ and $(\frac{\partial f}{\partial t})_{scatt}$ are equally important can be calculated by substituting into Eqn. (2.4) the following form for $(\frac{\partial f}{\partial t})_{e-e}$ (Conwell,1967) :

$$(\frac{\partial f}{\partial t})_{e-e} = \int \left[f(\vec{v}')f(\vec{v}_1') - f(\vec{v})\, f(\vec{v}_1)\right] |\mathcal{J}(\alpha, \vec{u})|^2 \, u \sin\alpha d\alpha d\gamma d^3 v_1 \qquad (2.27)$$

where $\vec{v}, \vec{v}_1$ are velocities of two electrons before collision.

$\vec{v}', \vec{v}_1'$ are velocities of the two electrons after collision.

$\vec{u} = \vec{v} - \vec{v}_1$

α is the angle through which the relative velocity of the two electrons are deflected due to collision.

γ is another angle specifying the orientation of $\vec{u}$ after the collision

$\mathcal{J}(\alpha, \vec{u})$ differential scattering cross-section for the collision.

The solution had been attempted only for a particular case, namely, for n-Ge at 78^{o} in the so called 'warm electron' range (Hasegawa, 1962)

2.4 With large carrier 'streaming'

So far only the case of extremely large carrier 'streaming' had been treated. Baraff (1964) and Dumke (1968) had assumed the distribution functions to be completely elongated in the direction of the applied field and applied them to discuss avalanche breakdown and ionisation processes. Evidently, these forms of distribution functions are not suitable for low fields.

Having discussed the various cases in Sections 2.1-2.4, one question would naturally arise as to whether the carrier-carrier scattering is predominant or not, whether the scattering processes contributing to $\left(\frac{\partial f}{\partial t}\right)_{scatt}$ is predominantly elastic and isotropic or not, and whether the electric field is high enough to cause large carrier 'streaming' or not, for a given physical situation. According to Fröhlich and Paranjape (1955), the carrier-carrier scattering would be predominant if the