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Hot Carriers and the Path Variable Method

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The Boltzmann transport equation describing a system of charge carriers in a strong electric field is transformed to a co-ordinate system determined by the collision-free trajectories of the particles. This formulation avoids the use of Legendre polynomial expansions and many of the approximations usually introduced in affecting a solution of the hot carrier problem.

A one dimensional integral equation is formulated for the energy distribution and is solved numerically. Energy distributions are computed for both n and p-type germanium at 77°K for several values of the electric field and are in excellent agreement with the experimental results.

§1. Introduction

The usual approach to the theory of transport phenomena in a strong electric field is based on an approximate solution of the Boltzmann transport equation. The steady state distribution function f(p) for the case of a uniform electric field E is determined by eq. (1).

$$eE \cdot \nabla_p f(p) = \widehat{Cf} \equiv \int dp' [f(p')T_{p'p} - f(p)T_{pp'}], \quad (1)$$

where p is the momentum vector, $T_{p,p'}$ is the transition rate between states p and p' due to collisions, and \hat{C} is the collision operator.

For spherical constant energy surfaces and isotropic scattering the distribution function can be expanded in Legendre polynomials in θ , the angle between the momentum vector and the applied electric field.

$$f(\mathbf{p}) = S_0(\varepsilon) + S_1(\varepsilon)P_1(\cos\theta) + S_2(\varepsilon)P_2(\cos\theta) \dots,$$

$$\varepsilon = \frac{p^2}{2 m^*}.$$
(2)

The insertion of this expansion into eq. (1) then leads to an infinite set of coupled integro-differential equations for the $S_n(\varepsilon)$. The standard approximation at this point is to neglect all but the two lowest order Legendre polynomials and to seek approximate solutions of the resulting equations.

In this paper we present a theory of hot carriers which does not employ Legendre polynomial expansions or arbitrary truncation procedures. In § 2 the Boltzmann equation is transformed to a co-ordinate system which follows the field dependent trajectories of the particles in the absence of collisions. This procedure transforms the Boltzmann equation into an integral equation for the distribution function. The case of hot carriers is treated in § 3, where we include energy losses due to optical phonons and momentum relaxation due to both acoustic and optical phonons. The resulting transport equation can then be reduced to a single one dimensional integral equation for the *isotropic* part of the distribution function. Having solved this equation, any of the terms in eq. (2) may be calculated by integration.

The kernel of this equation has been calculated numerically with the aid of an IBM 7044 and the integral equation is solved by an iterative procedure. The results for both n and p-type germanium are presented and discussed in §4 and are shown to be in excellent agreement with the experimental results.

§2. The Path Variable Method

We first consider the Boltzmann equation in the relaxation time approximation:

$$\left(\frac{\partial}{\partial t} + F \cdot \nabla_p + V \cdot \nabla_r\right) f(p, r, t) = -\frac{(f - f_0)}{\tau(p)}, \quad (3)$$

where $V = \nabla_p \varepsilon$ and f_0 is the equilibrium distribution. We now transform to a co-ordinate system determined by the collision free trajectories of the particles

$$r \rightarrow r^*(s)$$
, $p \rightarrow p^*(s)$, $t \rightarrow s$,

where:

$$\frac{d\mathbf{r}^*}{ds} = V, \quad \mathbf{r}^*(t) = \mathbf{r} \quad \text{and} \quad \frac{d\mathbf{p}^*}{ds} = F, \quad \mathbf{p}^*(t) = \mathbf{p}.$$
(4)

In these co-ordinates eq. (3) becomes:

$$\frac{df}{ds} = \frac{-f(s)}{\tau(s)} + \frac{f_0(s)}{\tau(s)} ,$$

which then yields

$$f(\boldsymbol{p},\boldsymbol{r},t) = \int_{-\infty}^{t} \frac{f_0(s)}{\tau(s)} \exp\left[-\int_{s}^{t} \frac{dy}{\tau(y)}\right] ds \,. \quad (5)$$

This generalization of Chambers' method^{1,2} will now be applied to the transport eq. (1), where one does not employ the relaxation time approximation. Introducing the transformations (4) in eq. (1) we obtain:

$$\frac{df}{ds} + \frac{f}{\tau(s)} = \int dp' f(p') T_{p'p^*(s)}; \frac{1}{\tau} \equiv \int T_{pp'} dp' \cdot (6)$$

This may now be transformed to the following:

$$f(\mathbf{p}) = \int f(\mathbf{p}') K(\mathbf{p}', \mathbf{p}) d\mathbf{p}' ;$$

$$K(\mathbf{p}', \mathbf{p}) = \int_{0}^{\infty} ds T_{\mathbf{p}', \mathbf{p} - Fs} \exp\left[-\int_{0}^{s} \frac{dy}{\tau(\mathbf{p} - Fy)}\right]. (7)$$

An alternate form of this equation, which will be used subsequently, is obtained by separating the distribution function f(p) into S_0 and A, its isotropic and anisotropic parts respectively, $f=S_0+A$. One then decomposes the collision term as follows:

$$\widehat{Cf} = \widehat{CS}_0 + \widehat{CA} = \widehat{CS}_0 - \frac{A}{\tau_M(\varepsilon)} , \qquad (8)$$

where the effect of collisions on the anisotropic part of the distribution function is described by an energy dependent relaxation time $\tau_M(\varepsilon)$.

The path variable transformations then yields:

$$f(\mathbf{p}) = \int_{0}^{\infty} ds \left[\widehat{CS}_{0} + \frac{S_{0}}{\tau_{M}(\varepsilon)} \right]_{\mathbf{p}-FS} \\ \times \exp\left[-\int_{0}^{s} \frac{dy}{\tau_{M}(\mathbf{p}-Fy)} \right],$$

where

$$F = eE. \tag{9}$$

§ 3. Phonon Scattering

In this section we apply the above formalism to the case of hot carriers, where we include energy losses due to optical phonons and momentum relaxation due to both acoustic and optical phonons. One can readily show in this case that the relaxation of the anisotropic part of the distribution function is indeed given by the usual relaxation time for *any* anisotropic distribution. This is rigorously true for optical phonon scattering and is valid in the limit of elastic acoustic phonon scattering.

Inserting the usual expressions for the transition probabilities in eq. (9) one can rewrite this equation as follows:

$$N(x) = \int_0^\infty dy N(y) \sum_{m=-1}^{+1} \alpha_m K_0(x, y+m\delta) ;$$

where

$$N(x) = \sqrt{x} S_0(x)$$
, $x = \frac{\varepsilon}{kT}$, $\delta = \frac{\hbar\omega_0}{kT}$, (10)

and

$$K_{0}(x, y) = \gamma \int_{|\sqrt{x} - \sqrt{y}|}^{\sqrt{x} + \sqrt{y}} \frac{dt}{t} \exp\left[-\sum_{n=-1}^{+1} \alpha_{n} \gamma g_{n}\right],$$

$$\gamma = \frac{\sqrt{2mkT}}{4 eE\tau_{A}(1)},$$

where

$$g_n = \text{Real part of} \left[\frac{a(t^2 + b^2)}{t} - \frac{(t^2 - a^2)(t^2 - b^2)}{2 t^2} \times \ln \left| \frac{t + a}{t - a} \right| \right]$$
(11)

$$a = \sqrt{y + n\delta} + \sqrt{x + n\delta}$$
, $b = \sqrt{y + n\delta} - \sqrt{x + n\delta}$.

N(x) is simply the number of carriers per unit energy range, $\tau_A(1)$ is the acoustic phonon relaxation time evaluated at x=1, and α_i is related to the ratio of optical to acoustical phonon deformation potential constants.

This formulation of the transport equation has thus resulted in an uncoupled equation for the isotropic part of the distribution function. Once eq. (10) is solved one may compute any of the $S_n(\varepsilon)$ in eq. (2) from the following relation:

$$S_n(x) = \int_0^\infty dy N(y) K_n(x, y)$$
(12)

where the kernel K_n is similar to that appearing in eq. (10).

The general procedure employed in solving eq. (10) was to compute the kernel numerically and then to solve this integral equation by iteration. The logarithmic divergence of the kernel at $x=y+m\delta$ was treated by analytic integration over a small range of y enclosing this singularity. N(y) was taken as constant throughout this interval, which was chosen to be extremely small compared to scale of variation of N. This typically amounted to taking N constant over an energy region of approximately $10^{-4} kT$, which clearly introduces negligible error.

The initial trial function, chosen to be a Maxwellian distribution, was inserted in the right hand side of eq. (10), thus generating a new energy distribution which was then re-introduced in the right hand side etc. Approximately 10 iterations sufficed to determine an energy distribution which satisfied eq. (10) to an accuracy greater than .01%.



Fig. 1A. Calculated heavy hole energy distribution for *p*-germanium at E=800 V/cm (dashed curve). Maxwellian distribution with same average energy (upper solid curve). Log of probability distribution (lower curve).



Fig. 1B. Calculated heavy hole energy distribution for *p*-germanium at E=926 V/cm (dashed curve). Maxwellian distribution with same average energy (upper solid curve). Log of probability distribution (lower curve).

§4. Results and Discussion

Figures 1 A and 1 B show the calculated energy distribution for *p*-type germanium at 77°K for E=800 V/cm and E=926 V/cm, respectively. The dashed curve in each case is the calculated energy distribution $N(x)=A\sqrt{x}S_0(x)$, where A is a normalization constant chosen such that $\int_0^{\infty} N(x)dx=1$. The upper solid curves represent Maxwellian distributions with the same average energy and are presented for comparison. The lower curves in each of these figures are the natural logarithm of the probability distribution $|\ln S_0(\varepsilon)|$. The parameters used are those given by Brown and Bray.³⁾

The relative impoverishment of high energy



Fig. 2A. Calculated energy distribution for *n*-germanium at E=1200 V/cm. (dashed curve). Maxwellian distribution with same average energy (upper solid curve). Log of probability distribution (lower curve).



Fig. 2B. Calculated energy distribution for *n*germanium at E=2000 V/cm (dashed curve). Maxwellian distribution with same average energy (upper solid curve). Log of probability distribution (lower curve).

carriers is readily seen from these results as in the non-Maxwellian nature of the energy distribution. It is seen from the $|\ln S_0|$ curves that the latter are fairly well approximated by two straight lines intersecting roughly at the optical phonon energy of 0.037 eV. Thus the energy distribution may be approximated by two Maxwellian distributions with different effective temperatures above and below the optical phonon threshold.

These features agree very well with the experimentally determined energy distributions for heavy holes in *p*-germanium. Pinson and Bray,⁴⁾ for example, have measured average heavy hole energies of \bar{z} =0.0218 eV and \bar{z} =0.0227 eV for E=800 V/cm and E=926 V/cm, respectively, while the present calculation yields \bar{z} =0.0216 eV and \bar{z} =0.0223 eV. The "kink" in the $|\ln S_0|$ curves at the optical phonon energy $\hbar\omega_0$ =0.037 eV has also been observed by Bray and Kumar.⁵⁾

While no direct measurements have been made of the drift velocity of heavy holes in *p*-germanium, Pinson and Bray⁴⁾ have presented results for $R=V_d$ (Total)/ $V_{\rm rms}$, the ratio of the total drift velocity (both light and heavy holes) to the r.m.s. heavy hole velocity, and argue that this ratio should be slightly larger than the corresponding ratio for the heavy holes alone. Here again we obtain excellent agreement with these results, the experimental values given at E=800V/cm and E=926 V/cm are R=0.5 and R=0.52respectively, which are indeed slightly larger than our calculated values for heavy holes of R=0.467and R=0.474.

Figures 2A and 2B show similar curves for *n*-germanium at 77°K for electric fields of 1200 V/cm and 2000 V/cm, respectively. The electric field is taken in the [100] direction in order to avoid the complications arising from "temperature" differences among the [111] oriented valleys. For this configuration, the relevant electronic mass is simply the conductivity mass $m^*=0.12 m_0$. The coupling constants used are those given by $J\phi$ rgensen, Meyer and Schmidt-Tiedemann.⁶⁾

It is seen from Fig. 2 that the distribution functions deviate relatively little from Maxwellian as compared to those in *p*-type germanium, this being due to relatively stronger coupling to optical phonons in the latter case. The calculated average energies and drift velocities for E=1200V/cm and E=2000 V/cm are $\bar{\varepsilon}=0.0416$ eV, $V_d=0.88\times10^7$ cm/sec and $\bar{\varepsilon}=0.10$ eV, $V_d=1.3\times10^7$ cm/sec respectively. The experimental values⁶¹ for the drift velocity at these two fields are $V_d\approx10^7$ cm/sec and $V_d\approx1.2\times10^7$ cm/sec respectively.

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References

- R. Chambers: Proc. Phys. Soc. (London) A65 (1952) 458.
- 2) H. Budd: J. Phys. Soc. Japan 18 (1963) 142.
- D. M. Brown and R. Bray: Phys. Rev. 127 (1962) 1593.
- W. E. Pinson and R. Bray: Phys. Rev. 136 (1964) A1449.
- 5) To be published
- M. H. Jørgensen, N. I. Meyer and K. J. Schmidt-Tiedemann: Proc. Int. Conf. Semiconductor Physics, Paris (1964) p. 457.

DISCUSSION

Reiss, H.: Isn't it important to consider collision integrals using non-singlet distribution function consideration when highly non-equilibrium distributions are involved.

Budd, H. F.: Although it would certainly be desirable to include many particle distributions in the theory, this is certainly an extremely difficult problem. Even a simple treatment based on particle-particle scattering and single particle distribution functions leads to intractable equations. The present calculation, which neglects these effects, is in excellent agreement with the experimentally determined average energies and drift velocities. There are however small differences in the shapes of the calculated and observed energy distributions. For example, the "kink" in the $|LnS_0|$ curves are observed to be less pronounced than our calculations indicate. This is probably due to our neglect of hole-hole scattering.

Landsberg, P. T.: The higher terms in the Boltzmann equation would involve electron or hole collisions and your paper is limitted in generality because these terms do not occur. We have considered the problem of the steady state distribution under optical injection and carrier collisions only. The procedure was somewhat similar to yours. An integral equation was solved by iteration. The results were given at Exeter Conference in 1962 (Proceedings, p. 857) and in greater detail by C. J. Hearn (Proc. Phys. Soc. 88 (1966) 407).

Budd, H. F.: The inclusion of higher order terms poses no formal problem and may be accomplished by the same transformations used in the present paper. The resulting equations are naturally far more complicated than our linear transport equation.