

Diffusion equation for hot electrons

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The diffusion equation for hot electrons is derived starting from the Boltzmann equation. It is shown that only under restricted conditions the equation may be simplified to a form analogous to the low-field form and a diffusion constant may be defined. The formula for the constant as derived for these conditions is found to be different from those given earlier. The formula indicates that the constant may be even negative at high fields in some materials and also that Monte Carlo calculations do not give its proper value. The hot-electron diffusion equation is also found to have an extra significant term, which does not occur in the low-field equation. Considering the conditions, required to be satisfied for the validity of the simplified form of the diffusion current, it is also concluded that the hot-electron diffusion cannot be analyzed by using the common phenomenological diffusion equation for the majority of diffusion experiments and hot-electron devices.

I. INTRODUCTION

The noise behavior^{1,2} and the space-charge propagation characteristics of hot-electron devices,³⁻⁵ such as Gunn diodes and avalanche diodes, being intimately related to the diffusion constant, the phenomenon of hot-electron diffusion is gaining increasing attention.⁶⁻¹⁰ The diffusion of holes in germanium and of electrons in silicon and gallium arsenide under hot-electron conditions have been experimentally studied.¹¹⁻¹⁴ However, the results do not show even qualitative agreement. The diffusion constant for holes¹¹ in germanium starts increasing from a field at which the conductivity does not show any significant hot-electron effect. In the case of silicon the constant in one experiment is found to decrease with increasing field,¹² whereas in another experiment it does not vary significantly with the field.¹⁴ On the other hand, in gallium arsenide the diffusion constant at first increases with the field and, passing through a maximum, ultimately decreases with increasing field.¹³

Theoretical results on hot-electron diffusion for germanium and silicon show that the diffusion constant should decrease with increasing field and passing through a minimum should increase at the end.¹⁰ The nature of the anisotropy in the diffusion constant as obtained theoretically is found to be different by different authors. In *p*-type germanium the diffusion constant $D_{||}$, for electrons diffusing parallel to the field, is found by Persky and Bartelink¹⁰ to be larger than the constant $D_{\perp}$, for diffusion perpendicular to the field. In silicon they find just the opposite nature of variation, $D_{\perp}$ being larger than $D_{||}$. On the other hand, the formula derived by Cheung and Hearn⁸ indicates that $D_{||}$ should be always less than $D_{\perp}$, being related, respectively, to the differential and cord mobility by the Einstein relation. Also, according to their results $D_{||}$ for Ge and Si should decrease with field at all fields. The Monte Carlo calculations⁷ of the

diffusion constant also do not agree well with experimental results. For silicon, the results of Monte Carlo calculations are in qualitative agreement with analytical results¹⁰ and are only in approximate agreement with experiments. For GaAs, the Monte Carlo results for $D_{\perp}$ only show some agreement,⁷ the results for $D_{||}$ being widely at variance with experiment.

In view of the existing discrepancy between the various formulas and experimental results, discussed above, it is worthwhile to reexamine the problem. In this paper we shall discuss the theory of hot-electron diffusion based on the Boltzmann equation, using a simple semiconductor model, and analyze the assumptions which have led to conflicting formulas and also to the discrepancy between theory and experiment.

II. BOLTZMANN EQUATION FOR THE DIFFUSION PROBLEM

We shall consider a nondegenerate semiconductor having a single valley, parabolic and isotropic band structure. We shall also assume that the electric field is uniform and the sample is neutral. The electron concentration gradient is assumed to be in the direction of the field.

The Boltzmann equation for the problem is

$$\frac{\partial f}{\partial t} = -\frac{\hbar k_x}{m^*} \frac{\partial f}{\partial x} - \frac{e\mathcal{E}}{\hbar} \frac{\partial f}{\partial k_x} + Lf, \quad (1)$$

where f is the distribution function, e , $\vec{k}$ and m^* are, respectively, the charge, wave vector, and effective mass of the electron. The electric field $\mathcal{E}$ is in the x direction. Lf is the collision term.

It is well known¹⁵ that an analytic solution of the above equation cannot be obtained unless some simplifying assumptions are introduced. However, considering the conflicting results reported in the literature it would appear that our understanding of the phenomenon is not clear even for the conditions for which the simplifying assumptions are applicable. Therefore, a study of the problem,

even introducing the necessary simplifying assumptions, and a study of the conditions required for the validity of the assumptions, is of interest.

The concentration of the carriers being nonuniform, the distribution function f will vary from point to point across the sample. But, as the carriers drift they get mixed up, and for a general solution we should consider the whole sample to constitute one system and attempt a solution of Eq. (1) with the proper boundary conditions in t and x . Such a solution is prohibitively difficult and has not been attempted so far. The problem may be simplified if we assume that at each point of the sample there is local dynamic equilibrium and we may define an f independent of the boundary conditions in x . This assumption will be satisfied if the sample is sufficiently long and the gain of energy and momentum by the drifting electrons at any point from the field, and due to drift, is balanced by the loss of the same to the lattice at a rate faster than the rate of displacement of the carriers. With this assumption, we may seek a solution of Eq. (1), determined by the conditions at each point, and the initial conditions need not be known. This assumption is basic to all hot-electron diffusion theory, including the Monte Carlo calculations.

Following the usual procedure, with the above mentioned assumption we may seek a solution for f in terms of a spherical-harmonic series. In materials with predominant optical phonon scattering, the carriers have a streaming motion under hot electron conditions, and for an acceptable representation the series for f should include at least two even terms. On the other hand, when randomizing collisions are strong the drifting motion is weak, and we may consider only the first term in the even part of f . We shall consider this case for the derivation of the formulas, noting that the formulas may be generalized to include the other case simply by inspection. We write for f

$$f = f_0(E, x, t) P_0(\cos\theta) + kf_1(E, x, t) P_1(\cos\theta), \quad (2)$$

where $P_0(\cos\theta)$ and $P_1(\cos\theta)$ are, respectively, the first and the second Legendre polynomials, θ is the angle between $\vec{k}$ and $\vec{\mathcal{E}}$, and E is the energy of an electron. Substituting expression (2) into Eq. (1), and using the orthogonal property of P_0 and P_1 , we get

$$\frac{\partial f_0}{\partial t} = -\frac{2}{3} \frac{E}{\hbar} \frac{\partial f_1}{\partial x} - \frac{2}{3} \frac{e\mathcal{E}}{\hbar} E^{-1/2} \frac{\partial}{\partial E} (E^{3/2} f_1) + Lf_0, \quad (3)$$

$$\frac{\partial f_1}{\partial t} = -\frac{\hbar}{m^*} \frac{\partial f_0}{\partial x} - \frac{e\hbar\mathcal{E}}{m^*} \frac{\partial f_0}{\partial E} + Lf_1. \quad (4)$$

We shall now assume that the concentration gradient is small so that we may separate f_0 and f_1 into two parts, i. e., an equilibrium part f_{0e}

+ $kf_{1e} \cos\theta$, representing the f in the absence of concentration gradient, and a perturbation part $f_{0p} + kf_{1p} \cos\theta$, introduced by the concentration gradient. Let n_0 be the carrier concentration corresponding to f_{0e} and n_1 be the excess concentration. Then we have

$$n_0 = \int f_{0e}(E) d\vec{k} \quad \text{and} \quad n_1(x, t) = \int f_{0p}(E, x, t) d\vec{k}.$$

The equilibrium parts satisfy these equations:

$$Lf_{0e} = \frac{2}{3} \frac{e\mathcal{E}}{\hbar} E^{-1/2} \frac{\partial}{\partial E} (E^{3/2} f_{1e}), \quad (5)$$

$$Lf_{1e} = \frac{e\mathcal{E}\hbar}{m^*} \frac{\partial f_{0e}}{\partial E}. \quad (6)$$

The perturbation parts, on the other hand, satisfy the complete Eqs. (3) and (4) and are functions of x , t , and E , the variables being not necessarily separable.

III. DIFFUSION CONSTANT FOR RELAXATION-TIME APPROXIMATION

To simplify the problem we shall seek solutions of Eqs. (3) and (4) assuming that the collisions are randomizing. It is well known that this assumption would be valid in elemental semiconductors. In compound semiconductors, the conditions do not permit us to make this assumption. However, deviation of the actual conditions from that assumed is not expected to make the qualitative features of the results inapplicable.

With the above assumption we may write

$$Lf_{1p} = -f_{1p}/\tau_m, \quad (7)$$

where τ_m is the momentum relaxation time. Using Eq. (7) we obtain, from Eq. (4),

$$\frac{\partial f_{1p}}{\partial t} = -\frac{\hbar}{m^*} \frac{\partial f_{0p}}{\partial x} - \frac{e\mathcal{E}\hbar}{m^*} \frac{\partial f_{0p}}{\partial E} - \frac{f_{1p}}{\tau_m}. \quad (8)$$

We assume that $\partial f_{1p}/\partial t \ll f_{1p}/\tau_m$. This assumption is satisfied if the frequency of the space-charge wave associated with the diffusion phenomenon is much less than $1/\tau_m$. In a drift experiment, the condition would be satisfied if the pulse rise-time is larger than τ_m . Values of τ_m are in the range 10^{-11} – 10^{-12} sec for most of the semiconductors.¹⁶⁻¹⁸ Hence this assumption would be satisfied for the experimental conditions up to the highest microwave frequencies and for a pulse rise time larger than 0.01 nsec.

Neglecting $\partial f_{1p}/\partial t$ in comparison to f_{1p}/τ_m , we obtain

$$f_{1p} = -\frac{\hbar\tau_m}{m^*} \frac{\partial f_{0p}}{\partial x} - \frac{e\mathcal{E}\hbar\tau_m}{m^*} \frac{\partial f_{0p}}{\partial E}. \quad (9)$$

Using Eq. (9) we find that the even part of the

perturbation in the distribution function satisfies the equation

$$\begin{aligned} \frac{\partial f_{0p}}{\partial t} = & Lf_{0p} + \frac{2}{3} \frac{e^2 \mathcal{E}^2}{m^*} E^{-1/2} \frac{\partial}{\partial E} \left(E^{3/2} \tau_m \frac{\partial f_{0p}}{\partial E} \right) \\ & + \frac{2}{3m^*} \frac{\partial}{\partial x} \left[E \tau_m \frac{\partial f_{0p}}{\partial x} + e \mathcal{E} \left(E \tau_m \frac{\partial f_{0p}}{\partial E} \right. \right. \\ & \left. \left. + E^{-1/2} \frac{\partial}{\partial E} (E^{3/2} \tau_m f_{0p}) \right) \right]. \end{aligned} \quad (10)$$

We note that the current density due to the excess carriers is given by

$$\begin{aligned} J = & - \frac{2e}{3m^*} \frac{\partial}{\partial x} \left(\frac{n_1 \int f_{0p} E^{3/2} \tau_m dE}{\int f_{0p} E^{1/2} dE} \right) \\ & - \frac{2e^2 \mathcal{E}}{3m^*} \frac{n_1 \int (\partial f_{0p} / \partial E) E^{3/2} \tau_m dE}{\int f_{0p} E^{1/2} dE}. \end{aligned} \quad (11)$$

At low fields the above expression for the current density gives two terms, one proportional to $\partial n_1 / \partial x$ and the other to n_1 and the diffusion constant is phenomenologically defined as the coefficient of $\partial n_1 / \partial x$. In the hot-electron problem, however, even for the simplified statement of the problem we get a more involved expression for J . It is evident from Eq. (10) that f_{0p} is dependent on $\partial n_1 / \partial x$ and also to its higher powers and derivatives. The expression for J , therefore, would include terms proportional not only to $\partial n_1 / \partial x$, but also to its higher powers and derivatives. Further, contributions to the term containing $\partial n_1 / \partial x$ will arise from the first term on the right hand side of Eq. (11) (corresponding to the low-field diffusion term) as well as from the second term (corresponding to the low-field drift term). In this context we may note that in the existing analysis of the hot-electron diffusion, these higher-order terms have been neglected without analyzing the conditions which justify this simplification. We shall discuss these conditions later. We discuss first the simplest result that we may derive from Eqs. (10) and (11).

IV. FORMULA FOR THE DIFFUSION CONSTANT, NEGLECTING HOT-ELECTRON EFFECTS OF CONCENTRATION GRADIENT

In order to evaluate J from Eq. (11) we are required to obtain f_{0p} by solving Eq. (10). As a first approximation we may neglect the derivatives with x and assume steady-state conditions, i.e., $\partial f_{0p} / \partial t = 0$. For this assumption we find that f_{0p} is defined by the same equation as defining f_{0e} , i.e., Eq. (5). Hence, it will differ from f_{0e} only through the normalizing constant. Replacing f_{0p} in Eq. (10) by f_{0e} , we get for the diffusion constant

$$D_{||} = \frac{2}{3m^*} \int f_{0e} E^{3/2} \tau_m dE / \int f_{0e} E^{1/2} dE. \quad (12)$$

The above formula is essentially the same as that derived by Persky and Bartelink.¹⁰ In the present derivation we have retained only one term in the even part of f . However, following the above procedure we may easily show that, for the general case, f_{0e} in expression (12) would be the complete even part of f and may include a number of terms depending on the material. The important point to be remembered is that the formula (12) for $D_{||}$ requires only the knowledge of the distribution function in the absence of the concentration gradient, and that $D_{||}$ may be accurately evaluated if this is known. If the analytic methods are inapplicable we may use the recently developed numerical methods¹⁹ for this purpose, to evaluate $D_{||}$ exactly.

V. FORMULA FOR THE DIFFUSION CONSTANT INCLUDING THE HOT-ELECTRON EFFECTS OF CONCENTRATION GRADIENT

The assumption on the basis of which expression (12) has been obtained may appear justified considering that $\partial n_1 / \partial x$ has been assumed to be small. However, the additional x -dependent terms appearing in f_{0p} from the solution of the complete equation gives a current component proportional to $\partial n_1 / \partial x$ and to $\mathcal{E}$, through the field term in J . This term may be comparable to the diffusion term in J . We may evaluate this additional term by solving Eq. (11), taking the detailed expression for Lf_{0p} . Since f_{0p} is then a function of t , x , and E , the complete solution is difficult. The method of successive approximation may be applied and a second-order approximate result may be obtained by replacing f_{0p} in the space and time derivatives by $n_1 f_{0e} / n_0$. However, as the present formulation is approximate in any case, we shall simplify the problem by assuming that f_{0e} , as well as f_{0p} , is Maxwellian and obtain an expression for f_{0p} from Eq. (10) by applying the energy-balance condition locally, i.e., by multiplying Eq. (10) by E and integrating over $\mathbf{k}$ space.

We may then write

$$f_{0e} = [n_0 \hbar^3 / (2\pi m^* k_B T_0)^{3/2}] e^{-E/k_B T_0} \quad (13)$$

and

$$f_{0p} = [n_1 / n_0 + (E/k_B T_0 - \frac{3}{2}) T_1 / T_0] f_{0e}, \quad (14)$$

where T_0 is the electron temperature in the absence of concentration gradient and T_1 is its change due to the diffusion current. Note that T_1 will vary with x and t .

Replacing f_{0p} in Eq. (10) by the function (14), multiplying by E , and integrating over all of $\mathbf{k}$ space we get

$$\frac{1}{n_0} \frac{\partial n_1}{\partial t} + \frac{1}{T_0} \frac{\partial T_1}{\partial t} = \frac{T_1}{T_0} \left[\phi + \frac{2e\mu_1 \mathcal{E}^2}{3k_B T_0} \left(\frac{\mu_2}{\mu_1} - 1 \right) \right] + \frac{2}{3} \frac{k_B T_0}{e} \frac{\partial}{\partial x} \left[\frac{\mu_2}{n_0} \frac{\partial n_1}{\partial x} + \frac{2\mu_3 - 3\mu_2}{2T_0} \frac{\partial T_1}{\partial x} - \frac{e\mathcal{E}}{k_B T_0} \left(\frac{n_1(\mu_1 + \mu_2)}{n_0} + \frac{(2\mu_3 - \mu_2 - 3\mu_1)T_1}{2T_0} \right) \right], \quad (15)$$

where

$$\mu_n = \frac{2e}{3n_0 m^*} \int \left(\frac{E}{k_B T_0} \right)^n \tau_m f_{0e} d\vec{k}$$

and

$$\phi = \frac{2}{3n_0 k_B T_0} \int EL \left(\frac{E}{k_B T_0} f_{0e} \right) d\vec{k}.$$

We may eliminate ϕ by using the expression for the differential mobility. Following the procedure detailed above we get for the differential mobility

$$\mu_d = \mu_1 - \frac{2e\mu_1 \mathcal{E}^2 (2\mu_2 - 5\mu_1)}{3\phi k_B T_0 + 2e\mathcal{E}^2 (\mu_2 - \mu_1)}. \quad (16)$$

Hence, we may write Eq. (15) as

$$\frac{1}{n_0} \frac{\partial n_1}{\partial t} + \frac{1}{T_0} \frac{\partial T_1}{\partial t} = \frac{T_1}{T_0} \left[\frac{2e\mu_1 \mathcal{E}^2}{3k_B T_0} \left(\frac{2\mu_2 - 5\mu_d}{\mu_1 - \mu_d} \right) \right] + \frac{k_B T_0}{3e} \frac{\partial}{\partial x} \left[\frac{2\mu_2}{n_0} \frac{\partial n_1}{\partial x} + \left(\frac{2\mu_3 - 3\mu_2}{T_0} \right) \frac{\partial T_1}{\partial x} - \frac{e\mathcal{E}}{k_B T_0} \left(\frac{2n_1(\mu_1 + \mu_2)}{n_0} + \frac{(2\mu_3 - \mu_2 - 3\mu_1)T_1}{T_0} \right) \right]. \quad (17)$$

Applying the energy-balance condition to Eqs. (5) and (6) we obtain

$$e\mu_1 \mathcal{E}^2 = 3k_B(T_0 - T_L)/2\tau_E, \quad (18)$$

where T_L is the lattice temperature. τ_E is the phenomenologically defined energy relaxation time, given by

$$1/\tau_E = [2/3k_B(T_0 - T_L)] \int EL f_{0e} d\vec{k} / \int f_{0e} d\vec{k}. \quad (19)$$

Evidently, τ_E is dependent on T_0 and T_L . The first term on the right hand side of Eq. (17) may, therefore, be replaced by

$$\frac{2e\mu_1 \mathcal{E}^2 T_1}{3k_B T_0^2} \left(\frac{2\mu_2 - 5\mu_1}{\mu_1 - \mu_d} \right) = \frac{T_1(T_0 - T_L)}{T_0^2 \tau_E} \left(\frac{2\mu_2 - 5\mu_1}{\mu_1 - \mu_d} \right). \quad (20)$$

Considering that the μ_n 's are all of the same order, we may neglect in Eq. (17) the space and time derivatives of T_1 if

$$\frac{1}{T_1} \frac{\partial T_1}{\partial x} \ll \frac{1}{\mu_1 \mathcal{E} \tau_E} \quad \text{and} \quad \frac{1}{T_1} \frac{\partial T_1}{\partial t} \ll \frac{1}{\tau_E}.$$

We then get for T_1

$$\frac{T_1}{T_0} = \frac{\tau_E(\mu_1 - \mu_d)}{(2\mu_2 - 5\mu_1)} \left[\frac{2k_B T_0}{3e} \left(\frac{\mu_2}{n_0} \frac{\partial n_1}{\partial x} - \frac{n_1 e \mathcal{E}}{n_0 k_B T_0} (\mu_1 + \mu_2) \right) - \frac{1}{n_0} \frac{\partial n_1}{\partial t} \right] \frac{T_0}{T_0 - T_L}. \quad (21)$$

We may now derive the diffusion equation by integrating Eq. (10) over all of $\vec{k}$ space. We obtain

$$\frac{1}{n_0} \frac{\partial n_1}{\partial t} = \frac{k_B T_0}{e} \frac{\partial}{\partial x} \left[\frac{\mu_1}{n_0} \frac{\partial n_1}{\partial x} + \frac{(2\mu_2 - 3\mu_1)}{2T_0} \frac{\partial T_1}{\partial x} - \frac{e\mathcal{E}}{k_B T_0} \left(\frac{n_1 \mu_1}{n_0} + \frac{(2\mu_2 - 5\mu_1)T_1}{2T_0} \right) \right]. \quad (22)$$

Replacing T_1/T_0 by expression (21) we get

$$\begin{aligned} \frac{\partial}{\partial t} n_1 - \frac{3a\mathcal{E}}{2} \frac{\partial n_1}{\partial x} + \frac{3ab}{2} \frac{\partial^2 n_1}{\partial x^2} &= \frac{\partial}{\partial x} \left[D_1 \left(1 - \frac{(\mu_1 - \mu_d)(\mu_1 + \mu_2)}{2\mu_1^2} \right) \frac{\partial n_1}{\partial x} - n_1 \mu_1 \mathcal{E} \right. \\ &\quad \left. + a\mathcal{E} D_2 \frac{\partial^2 n_1}{\partial x^2} + ab\mathcal{E}(\mu_1 + \mu_2) \frac{\partial^2 n_1}{\partial x^2} - abD_2 \frac{\partial^3 n_1}{\partial x^3} \right], \end{aligned} \quad (23)$$

where

$$a = \frac{\mu_1 - \mu_d}{2e\mu_1 \mathcal{E}^2} k_B T_0, \quad b = \frac{k_B T_0}{e} \frac{2\mu_2 - 3\mu_1}{2\mu_2 - 5\mu_1},$$

$$D_1 = \frac{\mu_1 k_B T_0}{e}, \quad D_2 = \frac{\mu_2 k_B T_0}{e}.$$

It is evident from Eq. (23) that, in spite of the simplifying assumptions, hot-electron diffusion is described by an involved equation. In fact, the phenomenological equation for the current density as used at low fields does not apply at high fields. The equation includes higher-order derivatives of n_1 . The analyses of hot-electron diffusion reported in the literature should, therefore, be considered approximate. The required condition for the valid-

ity of the approximations may be obtained by considering that the μ_n 's as well as the D_n 's are of the same order, and a is of the order of $\mu_1 \tau_E$. Hence, if $\partial n_1 / \partial x \ll n_1 / \mu_1 \mathcal{E} \tau_E$ we may neglect the higher derivatives and simplify Eq. (23) to

$$\frac{\partial}{\partial t} \left(n_1 - \frac{3a\mathcal{E}}{2} \frac{\partial n_1}{\partial x} \right) = \frac{\partial}{\partial x} \left(D_{||} \frac{\partial n_1}{\partial x} - n_1 \mu_1 \mathcal{E} \right), \quad (24)$$

where

$$D_{||} = D_1 [1 - (\mu_1 - \mu_d)(\mu_1 + \mu_2)/2\mu_1^2]. \quad (25)$$

Thus, we may define a hot-electron diffusion coefficient in agreement with the phenomenological definition under some restricted conditions, and the diffusion constant is then given by formula (25).²⁰ We should note, however, that we get an extra term in the diffusion equation involving $\partial^2 n_1 / \partial t \partial x$, which does not occur at low fields.

It may be recalled that D_1 is the diffusion constant obtained from expression (12) assuming a Maxwellian distribution function. The extra term appearing in formula (25) is the correction term due to the effect of the diffusion current on the distribution function. The magnitude of this term depends very much on the energy dependence of τ_m .

If we assume that τ_m varies as E^{-s} , we get

$$(D_{||} - D_1)/D_1 = -\frac{1}{2}(1 - \mu_d/\mu_1)(\frac{7}{2} - s). \quad (26)$$

The correction may be very significant when $\mu_d/\mu_1 \ll 1$. In fact, we find that for $S = \frac{1}{2}$, the fractional correction would be even larger than unity if $\mu_d/\mu_1 < \frac{1}{3}$. This condition would thus give a negative diffusion constant.²¹ However, it should be pointed out that this negative value may not be observable in practice due to the effect of the neglected terms and the extra terms on the left-hand side, which may be significant for the same conditions.

We should also note in this connection that in contrast to the conclusion of Cheung and Hearn,⁸ we do not obtain a modified Einstein relation for diffusion along the direction of the electric field. The assumption of the displaced Maxwellian distribution essentially would imply that $s = 0$, and for this condition we find that

$$D_{||} \neq \mu_d k_B T_0 / e.$$

This discrepancy may be due to the equation of the effect of diffusion current on the distribution by Cheung and Hearn⁸ with that due to a perturbation in the electric field, which does not appear to be justified according to the analysis presented here.

VI. DISCUSSION

The analysis given above indicates that only when $\partial n_1 / \partial x \ll n_1 / \mu_1 \mathcal{E} \tau_E$, we may use, for the analyses of hot-electron diffusion, and equation analogous to

the low-field phenomenological diffusion equation but having an extra term. In III-V compounds τ_E is of the same order as τ_m and lies in the range 10^{-11} – 10^{-12} sec.^{16–18} The maximum value of $\mu_1 \mathcal{E}$ being about 2×10^5 m/sec,¹⁵ we find that $(1/n_1) \times (\partial n_1 / \partial x)$ should be less than 0.5×10^6 m⁻¹. Thus, n_1 should not change substantially over a distance of 2 μ m, for the validity of the simplified equation. In the case of elemental semiconductors τ_E is larger by at least one order. Hence, this restriction would be more severe. Considering the conditions of the various experiments it appears that this restriction was not given any consideration. The interpretation of the experimental results on the basis of the low-field phenomenological equation, therefore, appears to be of doubtful significance and the discrepancies between the various experiments may arise from this source. It would also appear that the existing analysis of the diffusion effects in hot-electron devices, based on the low-field phenomenological equation for current density, should also be considered erroneous as the required condition is not obeyed in these devices, particularly in the microwave range. The proper method of analysis for the experimental conditions would be to use Eq. (23) and treat the coefficients of the various derivatives as unknowns to be determined by studying the frequency dependence of the diffusion current.

We also find that, even when the above-mentioned restrictive condition is obeyed, the effect on the diffusion constant of change in the distribution function caused by the concentration gradient is very significant. The formula of Persky and Bartelink¹⁰ would not, hence, represent the actual diffusion current. We also do not get a relation like the Einstein relation,⁸ relating the diffusion constant with the differential mobility.

In the light of the present discussion it is also of interest to consider the validity of the Monte Carlo results on the hot-electron diffusion constant. In the calculations reported in the literature,^{7,9} the trajectories of a single electron, under the influence of the electric field and affected by collisions, are simulated on the computer. The diffusion constant is then calculated using the formula

$$D_{||} = (\langle x_i^2 \rangle_{av} - \langle x_i \rangle_{av}^2) / 2T, \quad (27)$$

where the x_i 's are the distances travelled by the electron in the direction of the field in the sampling time T and $\langle \rangle_{av}$ denotes average value.

It may be proved, from statistical considerations,²² that if the distribution function of the electrons does not deviate appreciably from that corresponding to thermal equilibrium, expression (27) indeed gives the phenomenological diffusion constant. The formula may also be derived from the

solution of the low-field diffusion equation corresponding to a unit impulse input, which would give the probability of a displacement x in time T for an excess electron. As is well known, the distribution of the displacement is Gaussian with a mean-square deviation of $2DT$ as indicated by formula (27).

Under hot-electron conditions, however, the distribution function is not the thermal equilibrium function and it is significantly affected by the diffusion current. The diffusion equation is also different from the low-field equation. The validity of Eq. (27) for the calculation of $D_{||}$ is, therefore, questionable. Further, even if it is valid, the simulated electron trajectories would not represent actual displacements unless the effect of diffusion current is included. We may, hence, conclude that the presently available Monte Carlo results on $D_{||}$ do not represent the proper theoretical values. The value obtained from the Monte Carlo calculations may be equivalent to D_1 , i. e., the diffusion constant obtained by neglecting the effect of the diffusion current on the distribution function. Hence, the agreement observed by Persky and Bartelink¹⁰ between their results and Monte Carlo

calculations should not be taken as an indication of the correctness of their formula.

We should note in this connection that although the Monte Carlo calculations do not give the correct value of the diffusion constant, the results for the noise temperature²³ are expected to be valid as these are related to conditions without the concentration gradient.

It should also be mentioned that the correction term due to the diffusion current, although significant for diffusion along the direction of the field, would be of a smaller order for diffusion transverse to the field. The effect of the concentration gradient on the electron temperature for this case would be proportional to the square of the concentration gradient, whereas in longitudinal diffusion it is proportional to the product of the field and the concentration gradient. Hence, for transverse diffusion, results obtained by the Monte Carlo method,^{7,9} or from the formula of Persky and Bartelink,¹⁰ should be correct.

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