# Diffusion of Hot and Cold Electrons in Semiconductor Barriers*

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The electron current in a semiconductor at uniform lattice temperature $T_0$, with a nonuniform electric field distribution (e.g., a barrier layer), consists of terms arising from conduction, diffusion, and thermal diffusion. The first two terms involve the mobility and diffusion coefficient which are functions of the electron temperature $T$ or, more generally, depend on certain averages over the nonequilibrium, field-dependent electron energy distribution function. The third term is due to the electron temperature gradient and is analogous to conventional thermal diffusion of a gas in a temperature gradient. In conventional theory, which neglects electron heating or cooling, the mobility and diffusion coefficient are material constants and thermal diffusion is absent. Contrary to the case of uniform fields, $T$ is not a unique function of the local field; it also depends on the current and can only be determined by a simultaneous solution of the equations for current flow and conservation of energy with boundary conditions for a particular structure. As an example, a one carrier metal-semiconductor contact rectifier has been analyzed in detail including a discussion of the Peltier effect. In the barrier region $T$ is greater than $T_0$ (i.e., hot electrons) for a reverse bias but less than $T_0$ (i.e., cold electrons) for a forward bias. Computer solutions have been obtained for a Schottky barrier and electron scattering due to acoustic phonons only.

## 1. INTRODUCTION

THE drift velocity of electrons or holes in a semiconductor, under the influence of a uniform electric field, is proportional to the field strength $F$ only in the limit when $F$ tends to zero. In practice, an appreciable deviation of the carrier mobility, at room temperature, from its zero field limit requires a strong field. For example, in $n$-type germanium at room temperature, the electron mobility is halved for a field of about $3\times10^3$ v/cm.[1] (In the rest of this paper electrons will be considered specifically although the discussion applies equally well to holes.) The variation of the mobility arises from an increase of the average electron kinetic energy above the zero field, thermodynamic equilibrium value $\frac{3}{2}kT_0$ ($k$ is Boltzmann's constant and $T_0$ is the lattice temperature; only nondegenerate semiconductors will be considered). Thus if the field dependent average kinetic energy is expressed as $\frac{3}{2}kT(F)$, then the electron temperature[2] $T(F)$ is greater than $T_0$ and tends to it in the limit as $F$ tends to zero. The difference between $T$ and $T_0$ is determined by the condition that, in a steady current carrying state, the rate at which energy is supplied by the electric field to the electrons must be equal to the rate at which energy is transferred from the electrons to the lattice with electron lattice collisions. The electron mobility will be a function of $F$ through its dependence on $T$. This is known as the hot electron effect.[3]

The electron temperature has a precise significance only if the spherically symmetrical part of the electron distribution function in momentum space ($f_0$) retains its Maxwellian shape when a field is applied. In general this will not occur and the detailed shape of the distribution function ($f_0$) is required for calculations. In the remainder of this section the distribution function will be assumed to have a Maxwellian shape; the more general case will be discussed in Sec. 2.

Most of the existing experimental and theoretical work is concerned with the hot electron effect when a uniform electric field is applied to a homogeneous semiconductor. The current density is then proportional to the density of electrons and their drift velocity in the applied field. However, in structures which involve potential barriers, there will be an additional contribution to the current density, namely the diffusion current, which involves the spatial gradient of the electron density. In the usual theory, where the hot electron effect is neglected and the electron temperature is assumed to be equal to the lattice temperature (this will be referred to as the thermal equilibrium approximation or TEA), the current density $j$ is given by

$$j=en\mu F+eDdn/dx \tag{1}$$

in one dimension where $n$ is the electron density, $\mu$ is the mobility, $D$ is the diffusion coefficient, $-e$ is the charge on the electron, and $j$ is in the positive $x$ direction. In the TEA and for nondegenerate semiconductors it can be shown quite generally[4] that $D$ and $\mu$ are connected by the Einstein relation,

$$D/\mu=kT_0/e. \tag{2}$$

The question now arises: Is the TEA valid when Eq. (1) is applied to a barrier problem where the internal electric fields are comparable in magnitude to the uniform fields for which there is an appreciable hot electron effect? It has been argued in the past that since $\mu$ is already known as a function of $F$ from the hot electron studies, all that is required is a similar relation between

* A preliminary account of some of this work has appeared in Bull. Am. Phys. Soc. **6**, 107 (1961).

[1] W. Shockley, Bell System Tech. J. **30**, 990 (1951); E. J. Ryder, Phys. Rev. **90**, 776 (1953).

[2] This concept was first introduced by H. Fröhlich, Proc. Roy. Soc. (London) **A188**, 521 (1947).

[3] For reviews on this topic see J. B. Gunn, in *Progress in Semiconductors*, edited by A. F. Gibson (John Wiley & Sons, New York, 1957), Vol. 2, p. 246; and S. H. Koenig, J. Phys. Chem. Solids **8**, 227 (1959).

[4] P. T. Landsberg, Proc. Roy. Soc. (London) **A213**, 266 (1952).

$D$ and $F$.[5,6] However, as pointed out by Avak'yants,[7] this is an incorrect approach since when $j$ is zero, the electron temperature must everywhere be equal to the lattice temperature and $\mu$ and $D$ must be equal to their thermal equilibrium values, i.e., independent of the local value of $F$. In fact, just as in the uniform field case $\mu$, and also $D$, are functions of $T$. However, in a barrier region, $T$ is not a unique function of the local value of $F$ but is determined by the condition of conservation of energy in such a way that $T$ tends to $T_0$ when $j$ tends to zero.

In Sec. 2 it will be shown that the current density is actually given by

$$j=en\mu(T)F+ed[nD(T)]/dx, \tag{3}$$

where $\mu(T)$ and $D(T)$ are known functions of $T$, determined from the Boltzmann equation, for particular electron scattering mechanisms. [The general form of Eq. 3 also applies for a non-Maxwellian form of the distribution function[7] $f_0$; $D$ and $\mu$ are then defined in terms of integrals involving $f_0$, cf. Eqs. (16) and (17).] The Einstein relation, Eq. (2), is generalized to

$$D(T)/\mu(T)=kT/e, \tag{4}$$

so that Eq. (3) can also be written as

$$j=en\mu F+\mu kTdn/dx+enD^T dT/dx, \tag{5}$$

where

$$D^T=(k/e)\mu[1+d(\ln\mu)/d(\ln T)]. \tag{6}$$

The last term on the right hand side of Eq. (5) is then analogous to thermal diffusion or the Soret effect arising, in this case, from the electron temperature gradient.

Turning now to the evaluation of the electron temperature, let $nB(T)$ be the rate at which the electrons lose energy to the lattice by electron phonon collisions and $S(T)$ be the flux of energy in the positive $x$ direction. Then the conservation of energy for the electrons requires that

$$jF=nB(T)+dS(T)/dx, \tag{7}$$

where

$$S(T)=-\kappa(T)dT/dx-(j/e)\delta(T)kT. \tag{8}$$

$\kappa(T)$ is the thermal conductivity of the electrons and $\delta(T)kT$ is the average kinetic energy transported per electron arising from the current flow. (Here we are concerned with a one-carrier system and do not consider any effects due to carrier generation, recombination or trapping.) In Sec. 2, $B(T)$, $\kappa(T)$, and $\delta(T)$ will be determined by deriving Eqs. (7) and (8) from Boltzmann's equation [cf. Eqs. (21), (23) and (24)]. Equation (8) has the same form as the equation describing heat flow due to a lattice temperature gradient and a current in the TEA. The quantity $\kappa(T_0)$ is the usual electron thermal conductivity and $\delta(T_0)$ is the coefficient of the energy transport term which enters into the formula for the thermoelectric power,

$$\theta=(k/e)[(\zeta/kT_0)-\delta(T_0)], \tag{9}$$

where $\zeta$ is the Fermi energy. It will be shown that $\kappa(T)$ and the electrical conductivity $\sigma(T)$ obey a generalized Wiedemann, Franz, Lorenz, law:

$$\kappa(T)/\sigma(T)T=(k/e)^2\Delta(T), \tag{10}$$

where $\Delta(T)$ is a dimensionless number of order one, derived in Sec. 2 (Eq. 24), and $\Delta(T_0)$ is the usual result in the TEA.

The equations set up by Avak'yants[7] for the hot electron effect in barriers are also discussed in Sec. 2. Although Avak'yants starts with the non-Maxwellian form of the distribution function, as defined by the solution of Boltzmann's equation, he introduces several simplifications which finally leave a system of equations, equivalent to a special case of our Eqs. (3), (7), and (8).

To determine $T$, $n$, and $S$ as functions of $x$, for a given $j$ and $F$ from the three phenomenological differential equations [Eqs. (3), (7) and (8)] requires three independent boundary conditions. A fourth boundary condition is then sufficient for a unique relation between $j$ and a potential difference derived from $F$. To illustrate the solutions of these equations for a one-carrier system a Schottky barrier, semiconductor-metal contact, with neglect of image force for simplicity, will be considered in Sec. 4. The analysis requires numerical computations which have been carried out on an IBM 704 computer.

As a preamble to the detailed solutions, some formal integrations of the equations are carried out in Sec. 3. Integration of the energy balance equation [Eq. (7)] over various portions of the rectifier leads to a rather trivial generalization of the thermoelectric power but is of some interest in showing how the energy exchanges are distributed throughout the rectifier. Formal integration of the equation for the current (Eq. 3) enables us to discuss two previous approaches to the problem by Burgess[6] and by Landsberg[8] which are shown to be incorrect. Burgess used the experimental result that the electron drift velocity in $n$-type germanium is independent of $F$ for $F$ in excess of several kv/cm. He then assumed the TEA Einstein relation, leading to a diffusion constant inversely proportional to $F$. Using Eq. (1) he then obtained a volt-current characteristic, for an arbitrary potential variation in the barrier, which was equivalent to that for a Mott barrier (spatially constant barrier field) in the TEA. This approach is invalid since $\mu$ and $D$ cannot be unique functions of $F$, Einstein's relation in the TEA is not obeyed, and Eq. (3) rather than Eq. (1) should be used. An adequate criticism of Landsberg's approach can only be given in terms of the detailed analysis in Sec. 3.

Analytic solutions to the equations which are valid for weak currents are presented in Sec. 4; the computed results for arbitrary currents are discussed in Sec. 5.

[5] G. V. Gordeev, Fiz. Tvergdogo Tela **1**, 851 (1959) [translation: Soviet Phys.-Solid State **1**, 772 (1959)].
[6] R. E. Burgess, Proc. Phys. Soc. (London) **B66**, 430 (1953).
[7] G. M. Avak'yants, Zhur. Eksp. i Teoret. Fiz. **27**, 333 (1954).
[8] P. T. Landsberg, Proc. Phys. Soc. (London) **B68**, 366 (1955).

## 2. DERIVATION OF THE TRANSPORT COEFFICIENTS FROM BOLTZMANN'S EQUATIONS

The phenomenological equations stated in the previous section will now be derived from Boltzmann's steady state kinetic equation for the electron distribution function $f(\mathbf{p},x)$ in momentum ($\mathbf{p}$) and coordinate ($x$) space. The necessary modification of the usual hot electron theory for uniform fields requires calculations which are similar to those for current flow under a lattice temperature gradient in the TEA.[8,9] Hence, only a brief outline of the analysis need be given here. Boltzmann's equation can be written as[9]

$$eF\frac{\partial f}{\partial p_x}-\frac{p_x}{m^*}\frac{\partial f}{\partial x}+\left(\frac{\partial f}{\partial t}\right)_c=0, \tag{11}$$

where the first term is due to the field $F$, the second is due to diffusion ($m^*$ is the effective electron mass in the usual parabolic band model), and the third represents the effect of electron-phonon collisions. In general there will be additional terms to represent further scattering mechanisms, electron-hole generations and recombinations, etc. They will not be considered in the present paper.

Following the usual procedure, we expand $f(\mathbf{p})$ in spherical harmonics, viz.

$$f(\mathbf{p},x)=\sum_{\nu=0}^{\infty} f_\nu(E,x)P_\nu(\cos\theta), \tag{12}$$

where $\theta$ is the angle between $\mathbf{p}$ and the $x$ axis, $P_\nu(\cos\theta)$ are the Legendre polynomials, and only the first two terms are assumed to be important. Substituting into Eq. (11) gives

$$\frac{eFp}{m^*}\frac{\partial f_0}{\partial E}-\frac{p}{m^*}\frac{\partial f_0}{\partial x}-\frac{f_1(E)}{\tau(E)}=0, \tag{13}$$

for the $P_1(\cos\theta)$ terms. [Here, terms involving $f_2(E,x)$ have been neglected, cf. Appendix.] The particular form of the collision term which involves the relaxation time $\tau(E)$ only occurs for elastic collisions[10,11] or if the scattering matrix satisfies a certain symmetry relation.[12] (Detailed expressions for $\tau(E)$ in terms of the scattering matrix will be found in the references quoted.) In general however, the collision term involves an integral over $f_1(E)$ and the solution requires a variational technique.[9]

Substituting for $f_1$ into the expression for the current density,

$$j=-(e/m^*)\int p_x f(\mathbf{p})d^3p=-(e/3m^*)\int pf_1(p)d^3p, \tag{14}$$

leads to Eq. (3) where the electron density is

$$n=\int f_0 d^3p, \tag{15}$$

$$\mu=-\frac{2}{3}\frac{e}{m^*}\int_0^\infty \tau\frac{\partial f_0}{\partial E}E^{\frac{3}{2}}dE\Big/\int_0^\infty f_0E^{\frac{1}{2}}dE$$

$$=(e/m^*)\langle\tau[1+\tfrac{2}{3}d(\ln\tau)/d(\ln E)]\rangle, \tag{16}$$

$$D=(2/3m^*)\langle\tau E\rangle, \tag{17}$$

and the angular brackets denote averages with respect to $f_0$, namely

$$\langle G(E)\rangle\equiv\int f_0(E)G(E)d^3p\Big/\int f_0(E)d^3p$$

$$=\int_0^\infty f_0(E)G(E)E^{\frac{1}{2}}dE\Big/\int_0^\infty f_0(E)E^{\frac{1}{2}}dE. \tag{18}$$

The Einstein relation is thus generalized to

$$\lambda\equiv\frac{eD}{\mu}=-\int_0^\infty f_0\tau E^{\frac{3}{2}}dE\Big/\int_0^\infty(\partial f_0/\partial E)\tau E^{\frac{3}{2}}dE$$

$$=\frac{2}{3}\frac{\langle\tau E\rangle}{\langle\tau(1+\frac{2}{3}d(\ln\tau)/d(\ln E))\rangle}. \tag{19}$$

If we now assume a Maxwellian distribution function for $f_0$ i.e.,

$$f_0=nh^3(2\pi m^*kT)^{-\frac{3}{2}}\exp(-E/kT), \tag{20}$$

where $n$ and $T$ depend on $x$ but not on $E$, then $\lambda=kT$ (Eq. 4). For a non-Maxwellian form of $f_0$, Eq. (19) shows that $\lambda$ will again be related to a suitably defined average electron energy[7] which will however in general depend on the particular form of $f_0$ and value of $\tau(E)$.

The electron temperature $T$ in Eq. (20) can be determined by multiplying Eq. (11) by $E$ and integrating over momentum space. Then we obtain the conservation of energy Eq. (7), with

$$nB(T)=\int E(\partial f_0/\partial t)_c d^3p, \tag{21}$$

$$S(T)=(1/m^*)\int fEp_x d^3p=(1/3m^*)\int f_1Epd^3p. \tag{22}$$

$B(T)$ involves only the $f_0$ coefficient and can be evaluated for all scattering mechanisms, not necessarily elastic, if $f_0$ has the Maxwellian form [Eq. (20)]. Results for electron scattering by acoustic, polar, and nonpolar optical modes of lattice vibrations have been previously derived.[10,13] Substituting for $f_1$ from Eq. (13) into the expression for the energy flux $S(T)$, eliminating

[9] A. H. Wilson, *The Theory of Metals* (Cambridge University Press, New York, 1954), 2nd ed.
[10] R. Stratton, Proc. Roy. Soc. (London) **A242**, 355 (1957); **A246**, 406 (1958).
[11] H. Fröhlich, *Advances in Physics*, edited by N. F. Mott (Taylor and Francis, Ltd., London, 1954), Vol. 3, p. 325.
[12] C. Herring, Bell System Tech. J. **34**, 237 (1954).
[13] R. Stratton, J. Electronics & Control **5**, 157 (1958).

$F$ using Eqs. (3), (4) and (17), leads to Eq. (8), where

$$\delta(T)=\langle\tau E^2\rangle/\langle\tau E\rangle$$

and

$$\kappa(T)=(k/e)^2\Delta T n e\mu, \tag{23}$$

where

$$\Delta(T)=\left[\frac{\langle\tau E^3\rangle}{\langle\tau E\rangle}-\left(\frac{\langle\tau E^2\rangle}{\langle\tau E\rangle}\right)^2\right]\Big/(kT)^2 \tag{24}$$

is defined by Eq. (10).

In particular, for a relaxation time given by

$$\tau(E)=\tau_0(E/kT_0)^\nu, \tag{25}$$

where $\tau_0$ and $\nu$ are constant,

$$\mu=\frac{(\nu+\frac{3}{2})!}{(\frac{3}{2})!}\frac{e}{m^*}\tau_0\left(\frac{T}{T_0}\right)^\nu\equiv\mu_0\left(\frac{T}{T_0}\right)^\nu, \tag{26}$$

$$\Delta=\delta=\nu+\tfrac{5}{2},$$

where $\mu_0$ is the mobility in the TEA. For more complicated relaxation times however, e.g., when more than one scattering mechanism is of importance, $\delta$ and $\Delta$ will depend on $T$.

Removing the assumption of a Maxwellian form for $f_0$ would require the solution of Eq. (11) for the $P_0(\cos\theta)$ terms. This leads to a complicated partial differential equation for $f_0$ even for elastic collisions, when the collision term can be written as a differential expression.[10] Both $f_0$ and $f_1$ must be derived directly from Boltzmann's equation with boundary conditions appropriate to a particular structure.[14] Rather than deal with this very complicated problem we will discuss solutions based on the Maxwellian approximation in the rest of the paper. This may be a reasonably good assumption for a single, elastic, electron-phonon scattering mechanism where previous calculations[10] have shown that the mobility-field variation is not very sensitive to the precise shape of $f_0$. It would, however, only be a crude approximation for inelastic scattering[15] or for a combination of scattering mechanisms.[16] The possibility that predominant interelectronic collisions might actually induce a Maxwellian form for $f_0$[10,17,18] cannot apply in barriers, where the electron density is usually very low.

Avak'yants starts with Boltzmann's equation for $f_0$ and $f_1$ and assumes a relaxation time given by Eq. (25). By integrating these equations (with suitable multiplying factors) over momentum space he finds equations similar to Eqs. (3), (7), and (8) where the transport coefficients are defined in terms of the integrals

$$\chi^{(r)}=4\pi\int_0^\infty p^{r+2}F_0(p,x)dp,$$

where

$$f_0(p,x)\equiv n(x)F_0(p,x).$$

He then shows that $\chi^{(r)}/(\chi^{(2)})^{r/2}$, calculated with the appropriate distribution function for a strongly heated electron gas in a *homogeneous electric field*, is a pure number which depends on $r$ and the scattering index $\nu$. For each value of $r$ the ratio for various values of $\nu$ is close to that for $\nu=0$, the value that would occur in the TEA for all $\nu$. The important assumption made by Avak'yants is that each $\chi^{(r)}$ can be replaced by $(\chi^{(2)})^{r/2}$ times the factor $\chi^{(r)}/(\chi^{(2)})^{r/2}$ for $\nu=0$. He also sets $\chi^{(2)}/2m$ equal to $(3/2)kT$ which is equivalent to introducing the electron temperature $T$ via the Maxwellian form of $f_0$. Thus the final transport equations used by Avak'yants are equivalent to those based on a Maxwellian form for $f_0$ with $\nu=0$. It is difficult to judge the accuracy of this simplification since the derivation of the ratio $\chi^{(r)}/(\chi^{(2)})^{r/2}$ does not involve the correct space-dependent function $f_0(p,x)$. However, as we have previously observed, it is not unreasonable that the solution based on a Maxwellian form for $f_0$ is a good approximation (not necessarily with $\nu=0$) for a single, elastic electron-phonon scattering mechanism.

### 3. FORMAL INTEGRATION OF THE TRANSPORT EQUATIONS

For convenience the three phenomenological equations [Eqs. (3), (7), and (8)] will be rewritten in terms of the following reduced variables:

$$\begin{aligned}&x^*=x/L_D,\quad T^*=T/T_0,\quad \mu^*=\mu/\mu_0,\quad n^*=n/n_0,\\&F^*=FeL_D/kT_0,\quad V^*=eV/kT_0,\\&j^*=j[en_0\mu_0(kT_0/eL_D)]^{-1},\\&B^*(T^*)=B(T)[e\mu_0(kT_0/eL_D)^2]^{-1},\\&S^*(T^*)=S(T)[en_0\mu_0(kT_0/eL_D)^2L_D]^{-1},\end{aligned} \tag{27}$$

where $V$ is the electrostatic potential and the density $n_0$ and length $L_D$ are so far unspecified. (Subsequently $n_0$ will be taken as the bulk density of electrons and $L_D$ as the Debye length, corresponding to the donor density, for the Schottky barrier calculation.) For convenience, the asterisks on the reduced quantities will in the future be omitted; symbols without asterisks will refer to the reduced quantities unless otherwise stated. Then,

$$j=n\mu F+d(n\mu T)/dx, \tag{28}$$

$$jF=nB+dS/dx, \tag{29}$$

$$S=-\Delta n\mu T dT/dx-j\delta T. \tag{30}$$

These equations will now be applied to a one-dimensional $n$-type semiconductor-metal contact rectifier. The

[14] J. Yamashita, [Progr. Theoret. Phys. (Kyoto) **15**, 95 (1956)] has solved a similar problem, with additional terms due to electron multiplication in a $p$-$n$ junction, by separation of the variables $x$ and $E$ for $f_0$. This however presupposes that the electron temperature is independent of $x$, contrary to our results.

[15] T. N. Morgan, J. Phys. Chem. Solids **8**, 245 (1959).

[16] I. Adawi, Phys. Rev. **112**, 1567 (1958).

[17] H. Fröhlich and B. V. Paranjape, Proc. Phys. Soc. (London) **B69**, 21 (1956).

[18] J. Yamashita, Progr. Theoret. Phys. (Kyoto) **24**, 357 (1960).

formal volt-current characteristic[19] will be derived from Eq. (28) and compared with a previous calculation by Landsberg.[8] The energy exchanges for the rectifier will then be discussed in terms of Eq. (29).

It will be assumed that a plane $x=0$ can be defined which separates the bulk semiconductor ($x<0$) from the barrier region ($x>0$), where

$$n=1, \quad T=T_1 \quad \text{if} \quad x=0, \tag{31}$$

setting $n_0$ equal to the bulk electron density. (This assumption has recently been discussed by Macdonald[20] in the TEA.) $T_1$ differs from one by a small amount due to the electron heating in the bulk region. If the metal surface is at $x=L$ and the image force is neglected then

$$n=\exp(-V_D), \quad T=1 \quad \text{if} \quad x=L, \tag{32}$$

where $V_D$ is the reduced diffusion potential[19] (cf. Fig. 1). Here it is assumed that the electron temperature in the metal can never differ appreciably from the lattice temperature due to the high (degenerate) electron density. The effect of the image force will be considered later.

Integrating Eq. (28) and using the boundary condition [Eq. (31)] gives

$$n\mu T \exp\left(\int_0^x \frac{F}{T}dx'\right)-\mu_1 T_1 = j\int_0^x dx' \exp\left(\int_0^{x'} \frac{F}{T}dx''\right). \tag{33}$$

Inserting the boundary condition (Eq. 32) then gives[21]

$$j=\frac{\exp\left[-V_D+\int_0^L (F/T)dx\right]-\mu_1 T_1}{\int_0^L \exp\left[\int_0^x (F/T)dx'\right]dx}. \tag{34}$$

The barrier thickness $L$ is related to the reduced potential ($V_A$) applied across the barrier by the condition (cf. Fig. 1):

$$\int_0^L F dx = V_D - V_A. \tag{35}$$

Thus if $T$ and $F$ are known as functions of $x$, Eqs. (34) and (35) give the volt-current ($V_A-j$) characteristic of the barrier.

In the TEA, when $T=1$, Eq. (34) reduces to

$$j_0=[\exp(-V_A)-1]\Big/\int_0^L \exp(-V)dx, \tag{36}$$

where the zero of potential is taken at $x=0$. If the integral is approximated by noting that the integrand is large only near $x=L$ when $(V_D-V_A)\gg 1$, then

$$j_0 \approx F(L)\exp(-V_D)[1-\exp V_A]. \tag{36'}$$

In the particular case of a Schottky barrier, it is assumed that the space charge in the barrier layer is due to the completely ionized uniform distribution of donors while the charge due to the electrons is neglected. (See reference 20 for a recent discussion of this assumption.) If the length $L_D$, introduced in Eq. (27), is chosen as the Debye length,

$$L_D=(\epsilon k T_0/4\pi e^2 N)^{\frac{1}{2}}, \tag{37}$$

where $\epsilon$ is the dielectric constant and $N$ is the donor density (all these variables are unreduced), then the field and potential variations are given by

$$F=x, \quad V=-(1/2)x^2, \quad V_D-V_A=(1/2)L^2. \tag{38}$$

Substituting into Eq. (36) then gives

$$j_0=[\exp(-V_A)-1]\Big/\int_0^L \exp[(1/2)x^2]dx. \tag{39}$$

The integral has been tabulated in the form,

$$y(x)\equiv \exp(-x^2)\int_0^x \exp(t^2)dt, \tag{40}$$

by Lohmander and Rittsten.[22] Substituting into Eq. (39) then gives

$$j_0=\exp(-V_D)[1-\exp V_A]/2^{\frac{1}{2}} y((V_D-V_A)^{\frac{1}{2}}) \tag{39'}$$

using Eq. (38). This volt-current characteristic (first derived by Spenke[23]) is illustrated in Fig. 6 for the particular choice $V_D=10$. It will be compared with the results obtained in the next section when the TEA is not made. (Notice that $j$ is positive and $V_A$ is negative in the reverse direction.)

For an image force barrier, the two boundary conditions at the metal surface [Eq. (54)] will be replaced by two at the plane $x=L'$ near the metal surface which, after Landsberg[24] is defined by

$$V(L')=V_A; \tag{41}$$

i.e., it is the same potential as the bulk semiconductor conduction band edge for zero current. Then [cf. Eq. (32)]

$$n=1, \quad T=1 \quad \text{if} \quad x=L'; \tag{42}$$

[19] For a survey of the diffusion theory in the TEA, see the chapter on unipolar rectification theories by H. K. Henish, *Rectifying Semi-Conductor Contacts* (Clarendon Press, Oxford, 1957).

[20] J. R. Macdonald, Solid State Electronics, **5**, 11 (1962).

[21] Starting with (the incorrect) Eq. (1) instead of Eq. (3) leads to a result similar to Eq. (34), except that the factor $\mu_1 T_1$ in the numerator is absent while there is an additional factor $(1/\mu T)$ under the first integral sign of the denominator. With the assumption made by Burgess[5] ($T=1$, $\mu=v/F$, $v$ is constant), this gives $j=ve^{-V_D}(1-e^{V_A})/(1-e^{V_A-V_D})$. Apart from the coefficient $v$, this corresponds to setting $V=-Fx$ ($F$ is constant) in Eq. (36) for the TEA which gives the coefficient $(V_D-V_A)/L$.

[22] B. Lohmander and S. Rittsten, Kgl. Fysiograf. Sällskap. i Lund Förh. **28**, 45 (1958).

[23] E. Spenke, Z. Physik **126**, 67 (1949).

[24] P. T. Landsberg, Proc. Roy. Soc. (London) **A206**, 463 (1951).

so that, with Eq. (33),

$$j=\frac{\exp\left[\int_0^{L'}(F/T)dx\right]-\mu_1 T_1}{\int_0^{L'}dx\exp\left[\int_0^{x}(F/T)dx'\right]}. \quad (43)$$

Landsberg[8] starts with Eq. (1) instead of Eq. (3) and finds

$$j=\frac{\exp\left[\int_0^{L'}(F/T)dx\right]-1}{\int_0^{L'}dx(1/\mu T)\exp\left[\int_0^{x}(F/T)dx'\right]}. \quad (43')$$

(He actually retains the mobility $\mu$ and diffusion coefficient $D$ as unknown quantities and does not introduce the electron temperature $T$ explicitly.)

In the TEA, setting $T=1$, both equations give

$$j=[\exp(-V_A)-1]\Big/\int_0^{L'}dx\exp(-V). \quad (44)$$

Although this result is formally equivalent to Eq. (36) it corresponds to a different value of the upper limit and of $V(x)$. If the potential has a strong minimum in the barrier region at $x=b$, the integral can be replaced by Laplace's approximation,

$$\int_0^{L'}dx'\exp(-V)\approx[2\pi/V''(b)]^{\frac{1}{2}}\exp[-V(b)]. \quad (45)$$

Landsberg[24,25] has used Eqs. (44) and (45) to derive the volt-current characteristic in the TEA, for several types of potential barriers, including the image force correction. He also tried to simplify Eqs. (43′) in a similar way by making the assumption that[8] "the fractional variation of $\mu$ and $D$ (or in our case $T$) in the barrier is much less than the fractional variation of the electric field." Now

$$\int_0^{b}\left(\frac{F}{T}\right)dx'=-\int_0^{b}\frac{dV}{T}=-\frac{V(b)}{T(b)}-\int_0^{b}\frac{V}{T^2}dT. \quad (46)$$

Landsberg states that as a result of his assumption the last term in Eq. (46) may be neglected. It would, however, be more accurate to modify his assumption by replacing the electric field by the electronic potential. This is a far more stringent condition at the peak of the barrier where $dV/dx$ vanishes. Using Eq. (46) and Laplace's approximation then gives

$$\int_0^{L'}\frac{dx}{\mu T}\exp\left[\int_0^{x}\frac{F}{T}dx\right]\approx\frac{1}{\mu(b)T(b)}\left(\frac{2\pi T(b)}{V''(b)}\right)^{\frac{1}{2}}\exp\left(-\frac{V(b)}{T(b)}\right), \quad (47)$$

so that, substituting into Eqs. (43) and (43′),

$$j\approx\left(\frac{2\pi T(b)}{V''(b)}\right)^{\frac{1}{2}}\exp\left(\frac{V(b)}{T(b)}\right)\times\left\{\exp\left[\int_0^{L}\left(\frac{F}{T}\right)dx\right]-\mu_1 T_1\right\} \quad (48)$$

and

$$j\approx\mu(b)T(b)\left(\frac{2\pi T(b)}{V''(b)}\right)^{\frac{1}{2}}\times\exp\left(\frac{V(b)}{T(b)}\right)\left\{\exp\left[\int_0^{L'}\left(\frac{F}{T}\right)dx\right]-1\right\}. \quad (48')$$

Landsberg then argues that since $T(b)$ is evaluated at the potential minimum, where $F=0$, it should be equal to the thermal equilibrium value unity and therefore independent of applied voltage. Thus in the reverse direction, where the integral in Eq. (48′) becomes small with respect to one, the hot electron effect should be unimportant. However, it has already been shown in Sec. 1 that the electron temperature is not solely determined by the electric field but will certainly differ from the lattice temperature when a current flows. Thus even if the approximation to Eq. (46) is valid, $T(b)$ must still be calculated from the energy conservation equation. Our results in Sec. 5 show that $T$ actually varies extremely rapidly across the barrier. Although we did not include the image force in our calculation, it seems rather unlikely that Landsberg's assumption would be obeyed, so that even Eq. (48) itself is probably not applicable.

Turning now to the energy exchanges for the rectifier (with the image force again neglected), it is convenient to replace the mathematical discontinuity between the semiconductor and metal at $x=L$ by a continuous transition of phase from $x=L_1$, to $x=L_2$. Then integrating Eq. (29) from $x=0$ to $x=L_1$, gives the total rate at which energy is transferred to the lattice in the barrier region,

$$H\equiv\int_0^{L_1}nB(T)dx=j(V_D-V_A)+S(0)-S(L_1). \quad (49)$$

Similarly, for the transition region,

$$H_1\equiv\int_{L_1}^{L_2}nB(T)dx=-j(V_D-\zeta_0+\zeta_m)+S(L_1)-S_m(L_2), \quad (50)$$

[25] P. T. Landsberg, Proc. Roy. Soc. (London) **A206**, 477 (1951).

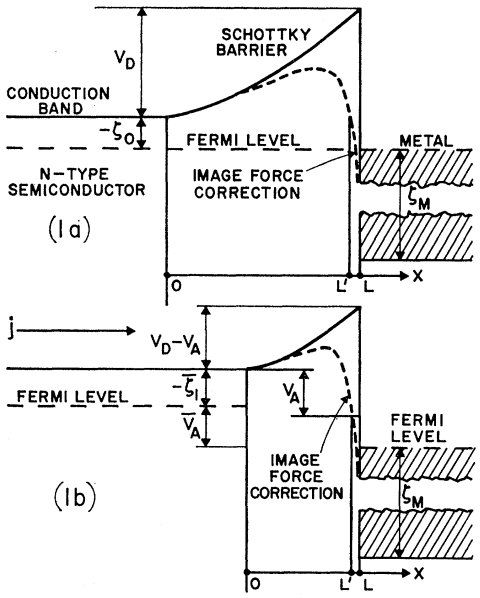


FIG. 1. Electron potential energy diagram for a metal $n$-type semiconductor contact rectifier. (a) Zero bias. (b) Bias $V_A$ applied in the forward direction.

where $\zeta_m$ is the reduced Fermi energy of the metal, $\zeta_0$ is the reduced Fermi energy of the semiconductor in the bulk region, for zero current, and

$$S_m=-j\delta_m \tag{51}$$

is the energy flux in the metal, where $T$ is assumed to be unity. Finally, integrating Eq. (51) from some large negative value of $x$ to $x=0$ gives

$$H_2\equiv\int^0 nB(T)dx=-jV_B-j\delta(\bar{T}_1)\bar{T}_1-S(0), \tag{52}$$

where $V_B$ is the voltage drop across the bulk region and the electron temperature far from the barrier tends to $\bar{T}_1$, given by

$$j^2=B(\bar{T}_1)\mu(\bar{T}_1), \tag{53}$$

using Eqs. (28) and (29) with $n$ and $T$ assumed independent of $x$. When $\bar{T}_1$, tends to one, i.e., as $j$ tends to zero, $B(\bar{T}_1)$ is proportional to $(\bar{T}_1-1)$ and $\mu(\bar{T})$ tends to the constant $\mu(1)$. Thus $\bar{T}_1$ differs from one by a term of order $j^2$ for small $j$. $\bar{T}_1$ will differ from $T_1$, introduced in Eq. (31), since $dT/dx$ is not zero at $x=0$. This difference will however be neglected in the next two sections since the calculated values of $dT/dx$ at $x=0$ are actually very small except for large currents in the forward direction. Adding Eqs. (49), (50), and (52) gives the total rate of energy transfer to the lattice for the rectifier:

$$H_T\equiv H+H_1+H_2=-j(\bar{V}_A+V_B)-j(\pi_m-\pi_1),$$

where

$$\pi_m=\zeta_m-\delta_m,\quad \pi_1=\bar{\zeta}_1-\delta(\bar{T}_1)\bar{T}_1, \tag{54}$$

and

$$\bar{V}_A=V_A+\bar{\zeta}_1-\zeta_0,$$

(cf. Fig. 1). Here $\bar{\zeta}_1$ is the reduced Fermi energy in the bulk semiconductor when a current flows; it is related to $\zeta_0$ by

$$\exp\zeta_0=\bar{T}_1^{\frac{3}{2}}\exp\bar{\zeta}_1 \quad\text{or}\quad \bar{\zeta}_1=\zeta_0-\tfrac{3}{2}\ln\bar{T}_1, \tag{55}$$

provided the electron density remains constant. Thus $\bar{V}_A$ is the change in Fermi level across the barrier region so that $-j(\bar{V}_A+V_B)$ is the Joule heating for the rectifier. The other contribution to lattice heating is due to the Peltier effect, where $\pi_m$ is the reduced Peltier coefficient of the metal and $\pi_1$ that for the semiconductor. The latter differs slightly from the usual expression $\pi_0$ in the TEA which has $\bar{T}_1$ replaced by unity. Since $\bar{T}_1-1$ goes to zero as $j^2$ [cf. Eq. (53)], $\pi_1$ differs from $\pi_0$ by a term of order $j^2$ in the limit of small currents.

The final Eq. (54) could have been obtained directly and is of course independent of the boundary conditions at $x=0$, $L_1$ and $L_2$. It is merely required that $T$ tends to $\bar{T}_1$ and unity in the semiconductor and the metal, respectively, far from the barrier. To evaluate the three contributions to $H_T$ separately requires a knowledge of the various values of $S$. This will be discussed in the next two sections.

Equations (49) to (55) also apply for the case of an image force barrier if $L_1$ is replaced by $L'$, $L_2$ is some point in the metal and $V_D$ is deleted from Eqs. (49) and (50).

## 4. LOW CURRENT LIMIT

The solution of the three reduced transport equations [Eqs. (28), (29) and (30)] will now be derived in the limit of small current densities. When the current density $j$ tends to zero, $T$ tends to unity, $S$ to zero, and $n$ to $\exp(-V)$. Also the quantities $\mu(T)$, $\delta(T)$, and $\Delta(T)$ have nonzero limits of 1, $\delta_0$ and $\Delta_0$, respectively, while $B(T)$ tends to zero. Thus, expanding $T$, $S$ and the product $n\mu T$ as power series in $j$,

$$T=1+jt,\quad S=js,\quad n\mu T=e^{-V}+j\sigma, \tag{56}$$

retaining terms of the first order in $j$ only. The coefficients $t$, $s$, and $\sigma$ which are functions of the position variable $x$ can be determined by substituting into Eq. (28), (29), and (30) from Eq. (56) and solving for the terms linear in $j$. For the rate of energy transfer $B(T)$ we make the assumption that

$$B(T)\to c(T-1)=jct,\quad\text{when}\quad T\to 1, \tag{57}$$

where $c$ is a coupling constant which depends on the strength and type of electron lattice scattering. Thus, carrying out the s ıbstitutions,

$$d\sigma/dx+F\sigma=1+Fte^V, \tag{58}$$

$$ds/dx+cte^{-V}=F, \tag{59}$$

$$\Delta_0e^{-V}dt/dx+s=-\delta_0, \tag{60}$$

with the boundary conditions [Eqs. (31), (32) and (35)]

$$t=0, \quad \sigma=0 \qquad \text{at} \quad x=0; \qquad (61)$$

$$t=0, \quad j\sigma=e^{-V_D}(1-e^{V_A}) \quad \text{at} \quad x=L. \qquad (62)$$

Eliminating $s$ between Eqs. (59) and (60) leads to the second order differential equation

$$\frac{d^2t}{dx^2}-F\frac{dt}{dx}-\frac{c}{\Delta_0}t=-\frac{Fe^{-V}}{\Delta_0}, \qquad (63)$$

which can in principle be solved for $t(x)$ if $F(x)$ is known. The function $\sigma(x)$ can then in turn be determined from the solution of Eq. (58) which is

$$\sigma=e^{V}\int_0^x (e^{-V}+Ft)dx, \qquad (64)$$

while $s$ can be determined from either Eqs. (59) or (60). Combining Eq. (64) and the boundary condition (62) leads to the voltage-current characteristic,

$$j=j_0[1+\beta]^{-1}, \qquad (65)$$

where

$$\beta=\int_0^L Ftdx \Big/ \int_0^L e^{-V}dx \qquad (66)$$

and $j_0$ is the expression for $j$ in the TEA given by Eq. (36). The correction term $\beta$ is a function of the applied potential $V_A$ which can be derived once the solution for $t$ of Eq. (63) is known.

As an example, the case of a Schottky barrier [cf. Eq. (38)] will now be considered. The solution of Eq. (63) is then[26]

$$t=\frac{x}{2\Delta_0 a}\left[\frac{\Phi(a,\tfrac{3}{2};-\tfrac{1}{2}x^2)}{\Phi(a,\tfrac{3}{2};-\tfrac{1}{2}L^2)}-1\right]\exp(\tfrac{1}{2}x^2), \qquad (67)$$

where

$$a=1-\tfrac{1}{2}c/\Delta_0 \qquad (68)$$

and $\Phi(a,c;x)$ is the confluent hypergeometric function. Substituting into Eq. (66) gives, after some manipulation,[26]

$$\Delta_0\beta(a, V_D-V_A)$$

$$=\frac{1}{2a}\left[1-\frac{\Phi(1+a,\tfrac{3}{2};-\tfrac{1}{2}L^2)}{\Phi(1,\tfrac{3}{2};-\tfrac{1}{2}L^2)\Phi(a,\tfrac{3}{2};-\tfrac{1}{2}L^2)}\right] \qquad (69)$$

$$\approx 1+2(2a-1)/L^2+5(4a^2-1)/L^4+O(L^{-6}). \qquad (69')$$

The dependence[27] of $\beta\Delta_0$ on $c/\Delta_0$ is illustrated in Fig. 2

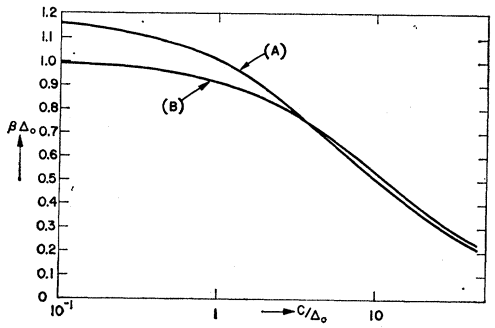


FIG. 2. The dependence of the correction term $\beta(a, V_D-V_A)$ on $c/\Delta_0$ [cf. Eqs. (65) and (69)]. Curve A refers to the present calculations and curve B to the result of Avak'yants.[7]

(curve $A$) for the case $(1/2)L^2=(V_D-V_A)=10$. From the asymptotic properties of the confluent hypergeometric function it can be shown that $\beta$ tends to zero as either $c$ or $\Delta_0$ tend to infinity for all values of $L$. When $c/\Delta_0$ tends to zero, $\beta\Delta_0$ tends to 1.183.

Using the solution for $t$, the other variables $s$ and $\sigma$ can be evaluated. In particular we find that the rates of energy transfer [Eqs. (49), (50), and (52)] are given by

$$H/j=\tfrac{1}{2}L^2+\tfrac{1}{2}[\Phi(a,\tfrac{1}{2};-\tfrac{1}{2}L^2)-1]/\Phi(a,\tfrac{3}{2};-\tfrac{1}{2}L^2), \qquad (70)$$

$$H_1/j=-\tfrac{1}{2}L^2+\pi_0+\tfrac{1}{3}L^2\Phi(1+a,\tfrac{5}{2};-\tfrac{1}{2}L^2)/\Phi(a,\tfrac{3}{2};-\tfrac{1}{2}L^2), \qquad (71)$$

$$H_2/j=[\{\Phi(a,\tfrac{3}{2};-\tfrac{1}{2}L^2)\}^{-1}-1]/2a, \qquad (72)$$

and

$$H_T=H+H_1+H_2=j\pi_0, \qquad (73)$$

considering only terms linear in $j$ and setting $\zeta_m$ approximately equal to $\delta_m$, i.e., neglecting the Peltier coefficient of the metal with respect to that of the semiconductor ($\pi_0$). The fact that Eqs. (70), (71), and (72) are consistent with Eq. (73) can easily be verified[26] with the aid of the recurrence relations for the confluent hypergeometric functions.

The dependence of $(H/j)$, $(H_2/j)$, and $\pi_0-(H_1/j)$ on $c/\Delta_0$ is illustrated in Fig. 3 for the case $(1/2)L^2=V_D-V_A=10$. For a current in the reverse direction ($j$ is positive), the rectifying contact as a whole is cooled at the rate $j\pi_0$ ($\pi_0$ is negative). The interface is cooled at a

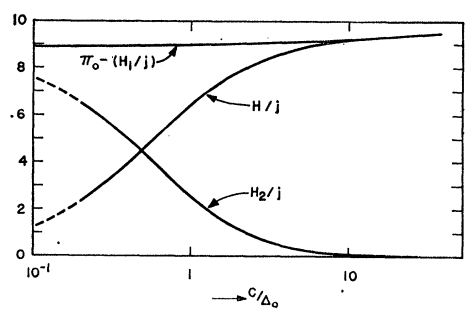


FIG. 3. The dependence of various rates of energy transfer, in reduced units, on $c/\Delta_0$ [cf. Eqs. (49), (50), and (52)].

[26] Equation (63) can be solved by making the substitution $t=u\exp(\frac{1}{2}x^2)$ and using the solution of the resulting standard equation given by A. Erdelyi, *Higher Transcendential Functions* (McGraw-Hill Book Company, Inc., New York, 1953). The various integrals and recurrence relations required for the derivation of Eqs. (69)–(73) will also be found in this compilation.

[27] For a recent table of numerical values see L. J. Slater, *Confluent Hypergeometric Functions* (Cambridge University Press, New York, 1960).

rate in excess of $j\pi_0$ which varies only slightly (from $8.94j$ to $10j$) as $c/\Delta_0$ goes from zero to infinity. This excess cooling is balanced by the rate at which the barrier region ($H$) and the bulk region ($H_2$) are heated. The former is dominant for large $c/\Delta_0$ and the latter for small $c/\Delta_0$. If the current is in the forward direction, the sign of $j$ and all the other quantities is reversed. In particular, $H$ is then negative since the electron temperature in the barrier region is then less than the lattice temperature, i.e., "cold" electrons. Physically this arises since the energy required by the electrons, when climbing up the potential barrier, must be supplied by the lattice.

To determine the range of $j$ values for which the low-current solution is an adequate approximation requires estimates of the second order terms in the power series expansions of Eq. (56). This leads to a set of differential equations which is more complicated than the original transport equations. Thus, the range of application of the low current solution will be determined by comparing with the computed solutions, for arbitrary $j$, presented in the next section.

Avak'yants also considered the low-current limit but only derived the correction to the TEA zero-bias resistance. Although he specified a Schottky barrier, he actually assumed a constant field in the barrier region whose thickness was correctly deduced from the barrier height. After some considerable manipulation, his final result[7] [Eq. (53)] can be rewritten as

$$\Delta_0\beta=2\{1+(c/\Delta_0V_D)+[1+(2c/\Delta_0V_D)]^{\frac{1}{2}}\}^{-1}, \quad (74)$$

where $\Delta_0=\frac{5}{2}$ corresponding to $\nu=0$. This result gives curve $B$ in Fig. 2; it deviates appreciably from our calculated curve $A$. When $c/\Delta_0$ tends to zero, $\Delta_0\beta$ tends to one.

### 5. RESULTS OF THE NUMERICAL ANALYSIS

The solution of the three reduced transport equations [Eqs. (28), (29), and (30)] for arbitrary values of the current $j$ must be carried out numerically. It then becomes necessary to specify a particular barrier profile and electron lattice scattering mechanism at the outset. As an example, computer solutions have been obtained for the following illustrative example of a one-dimensional semiconductor metal contact rectifier.

(a) Schottky barrier [cf. Eq. (38)] with neglect of the image force correction. It will be shown that inclusion of the latter would considerably complicate the procedure adopted for the numerical solutions.

(b) Reduced diffusion potential $V_D=10$. This is the only parameter required to specify the barrier for the numerical calculation; the value selected is typical of experimental values quoted in the literature.

(c) Electron scattering by acoustic modes of vibration only; i.e., $\nu=-\frac{1}{2}$ in Eq. (25). Then, from Eq. (26) and reference 10,

$$\mu=T^{-\frac{1}{2}}, \quad \Delta=\delta=2, \quad B=cT^{\frac{1}{2}}(T-1), \quad (75)$$

where the dimensionless coupling constant $c$ is given[10] as

$$c=\frac{32}{3\pi}\left[\frac{s}{\mu_0}\frac{eL_D}{kT_0}\right]^2=12\left(\frac{m^*s^2}{kT_0}\right)\left(\frac{L_D}{l}\right)^2 \quad (76)$$

in unreduced quantities. Here $s$ is the velocity of sound, $m^*$ the effective electron mass and $l$ the mean free path. Equations (28), (29), and (30) would be considerably more complicated for a relaxation time which is not proportional to a power of the electron energy. For example, although it is possible to obtain an analytic expression for $B(T)$ when electron scattering is due to both acoustic and nonpolar optical modes of vibrations,[13] the quantities $\mu(T)$, $\delta(T)$, and $\Delta(T)$ involve numerical integrations.

(d) Coupling constant $c=10$ (i.e., $a=-1.5$). With values of $s$ typically about $5\times10^5$ cm sec$^{-1}$, the value of $c$ can be written as

$$c=0.066(m^*/m)(300/T_0)(L_D/l)^2, \quad (76')$$

where $m$ is the free electron mass. The range of possible values for $c$ is bounded from below by the condition (cf. Appendix)

$$Fel\ll kT \quad \text{or} \quad (L_D/l)\gg[2(V_D-V_A)T_0/kT^2]^{\frac{1}{2}}, \quad (77)$$

in unreduced quantities [using Eq. (38)], and from above by the condition

$$\mu\gg(2/3)e\hbar/m^*kT, \quad (78)$$

also in unreduced quantities. (The latter condition, given by Fröhlich and Sewell,[28] is obtained by inserting the relaxation time into Heisenberg's uncertainty relation.) Combining Eqs. (76), (77), and (78) leads to

$$24\left(\frac{m^*s^2}{kT}\right)\left(\frac{V_D-V_A}{kT}\right)\ll c\ll\frac{24}{\pi}\left(\frac{m^*sL_D}{\hbar}\frac{T}{T_0}\right)^2, \quad (79)$$

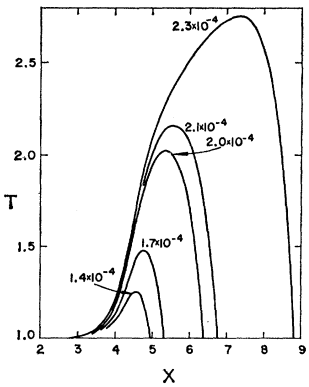


FIG. 4. The variation of the reduced electron temperature $T$ through the barrier region for various values of the current density $j$, in the reverse direction, marked on the figure. The point $x=0$ (not shown in the figure) corresponds to the foot of the barrier, i.e. where the bulk and barrier regions join. The value of $x$ where $T=1$ at the right-hand side of each curve (i.e., at the metal-semiconductor contact) gives the barrier thickness.

[28] H. Fröhlich and C. L. Sewell, Proc. Phys. Soc. (London) **74**, 643 (1959).

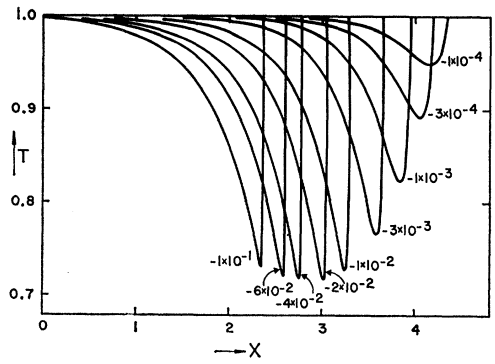


FIG. 5. The variation of the reduced electron temperature $T$ through the barrier region for various values of the current density $j$, in the forward direction, marked on the figure. The point $x=0$ corresponds to the foot of the barrier, i.e. where the bulk and barrier regions join. The value of $x$ where $T=1$ at the right-hand side of each curve (i.e., at the metal-semiconductor contact) gives the barrier thickness.

or, using Eq. (37),

$$0.13\left(\frac{m^*}{m}\frac{300}{T_0}\right)\left(\frac{V_D-V_A}{kT}\right) \ll c \ll \frac{3.3\times10^{17}}{N}\left(\frac{m^*}{m}\right)^2\left(\frac{T_0}{300}\right)\left(\frac{T}{T_0}\right)^2, \quad (79')$$

taking $s=5\times10^5$ cm sec$^{-1}$, $\epsilon=16$, and $N$ in cm$^{-3}$. The value $c=10$ selected will satisfy these inequalities for reasonable values of the other parameters. Some results have also been obtained for $c=2.5\times10^{-3}$ (i.e., $a\approx1$) which would require improbably low values of the effective mass, say less than about $2\times10^{-3}$ m. (This value of $c$ actually corresponds to $n$-type Ge, assuming acoustic scattering only and taking $N=10^{16}$ cm$^{-3}$.) It is nevertheless of interest to compare these results with those for the main calculation due to the large difference between the two values of $c$ selected.

The equations were programmed for an IBM 704 computer following the Runge-Kutta procedure.[29] For convenience the rapidly varying quantities $n$ and $T$ were replaced by new variables $\phi$ and $\theta$ defined by the relations:

$$n\mu T\equiv\exp(V-\phi) \quad \text{and} \quad T-1=\theta\exp(-V).$$

A two-point boundary problem has to be solved. Starting at $x=0$, the foot of the barrier, with the known values of $\phi$ and $\theta$ (or $n$ and $T$) for a given $j$ [Eqs. (31) and (53)] and a guess at the value of $s$, the equations are integrated for increasing $x$ until $\theta=0$ (or $T=1$) at the metal interface.[30] The corresponding values of $\phi$ and $x$, i.e., $V_A$ and $L$ must then satisfy the relation $V_A+\frac{1}{2}L^2=V_D$ [Eqs. (32) and (38)]. By iteration the correct choice of $s(0)$, for a given $j$, which leads to the chosen value of $V_D$, can then be found.

Inclusion of the image force correction would lead to a term proportional to $(L-x)^{-2}$ in the expression for $F(x)$. Since however, the barrier thickness $L$ for a given $j$ is not known *a priori*, it would have to be determined by trial and error just as $s(0)$. The procedure would then involve selecting $s(0)$ and $L$ such that when the equations were integrated from 0 to $L$, $\theta(L)=0$ and $\phi(L)=V_A=V_D-\frac{1}{2}L^2$. Clearly, a considerable amount of iteration would be required to find the correct solutions.

The results of the calculation are illustrated in Figs. 4 through 7. The variation of the reduced electron temperature $T$ through the barrier region, for various values of the current $j$, is shown in Figs. 4 and 5. The position of the foot of the barrier ($x=0$) is not included in Fig. 4 for the reverse direction since $T$ only deviates appreciably

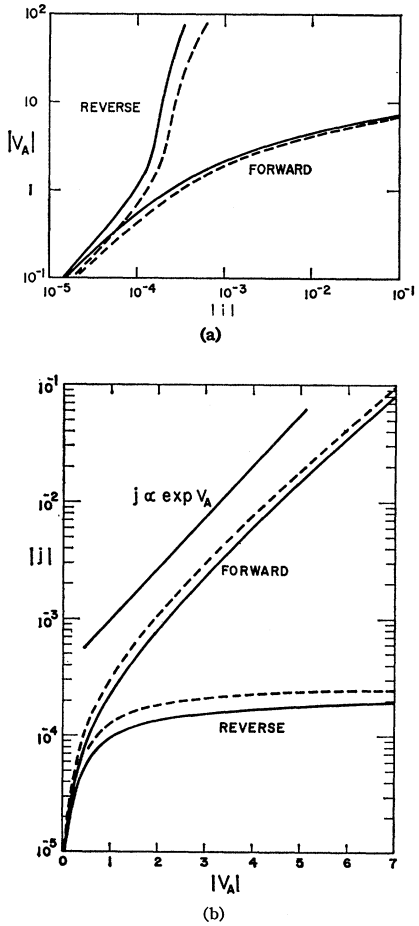


FIG. 6. The computed volt current characteristics (full line curves) for a Schottky barrier rectifier ($a-\ln|j|$ vs $\ln|V_A|$, $b-\ln|j|$ vs $V_A$). The dashed curves were calculated with the TEA using Eq. (39). A straight line whose slope corresponds to the simplified expression $-j\propto\exp V_A$ for the forward current has been included in the figure for comparison with the computed curves.

[29] The method is analogous to that described in reference 20. The author is indebted to Dr. J. Ross Macdonald for the IBM 704 program.

[30] For currents in the forward direction, $\theta$ decreases from a small positive value at $x=0$, passes through zero to minimum and then increases to $u=0$ again. It is the second position where $u=0$ which gives the barrier thickness.

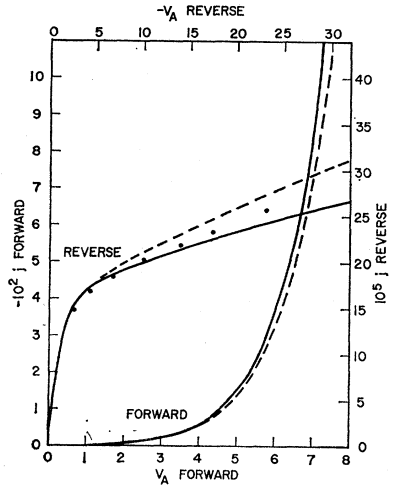


FIG. 7. Linear plot of the computed Schottky barrier rectifier voltage-current characteristic (full line curve). The dashed curve represents $j_0[1+\beta(-1.5, 10)]^{-1}$, the low-current solution [Eq. (65)], where $j_0$ is the TEA solution [Eq. (30)]. The points represent the more accurate low current solution, $j_0[1+\beta(-1.5, 10-V_A)]^{-1}$, calculated only for the reverse direction by use of the asymptotic expansion, Eq. (69′).

(say by 2%) when $x$ exceeds about 3. However, for currents in the forward direction (cf. Fig. 5), $T$ deviates appreciably already near $x=0$ due to the higher currents that can flow. Whereas the maximum electron temperature in Fig. 4 appears to increase continuously as $j$ increases, the minimum electron temperature in Fig. 5 at first decreases but then reaches a lowest value of 0.715 for $j$ equal to about $-4\times10^{-2}$. The electron temperature gradient becomes very large near the metal semiconductor interface, i.e., the position where $T=1$ at the right hand side for each curve in Figs. 4 and 5. It is equal to about 4 for the highest current plotted in Fig. 4 and exceeds 100 for currents in excess of $-2\times10^{-2}$ in the forward direction. These large values are no doubt connected with the discontinuity in potential of the Schottky barrier. Inclusion of the image force correction would lead to a more gradual variation of $T$ near the metal semiconductor interface.

In the Appendix it is shown that besides inequality (77), the electron temperature must also satisfy

$$(1/T)dT/d(x/L_D)\ll L_D/l, \tag{80}$$

in unreduced quantities. With $c=10$, $(L_D/l)$ is about $12(m/m^*)^{\frac{1}{2}}$, using Eq. (76′). Thus the condition is likely to be violated for large currents in the forward direction. Examination of the computed results reveals that for a given $(L_D/l)$, the other conditions given in the Appendix will also be obeyed up to those current levels for which inequality (80) is still satisfied. [An exception is the third member of inequality (A9) which will not be satisfied, for any $j$, in the immediate vicinity of the maximum and minimum values of $T$; this will not, however, introduce any appreciable errors.]

The computed volt-current characteristic is compared with that for the TEA [cf. Eq. (39′)] in Figs. 6 and 7. The zero bias resistance is increased by the factor $1+\beta(-1.5, 10)=1.338$ [cf. Eq. (69)] above the TEA value. Figure 7 shows that the computed current density $j$ actually differs appreciably from $j_0/[1+\beta(-1.5, 10)]$ only for voltages in excess of 4 in both directions. This can be verified by displacing the two sets of curves, in the double logarithmic plot (Fig. 6), along the $|j|$ axis. Better agreement can be obtained by using the full expression $j_0/[1+\beta(1.5, 10-V_A)]$ derived for this low-current region. This is exemplified by the solid points in Fig. 7 which have been derived with the use of Eq. (69′). The wide range of application of the solution for low currents was unexpected; its demonstration is an important result of the numerical analysis. It seems reasonable that the low-current solutions for barriers of different shapes will also have a fairly extensive range of validity although this has not been tested. This conjecture is supported by numerical solutions of the transport equations with the coupling constant $c$ taken as $2.5\times10^{-3}$. They were qualitatively similar to those for $c=10$. In particular, the low-current solution was adequate for voltages of up to $-4$ in the reverse and 5 in the forward direction.

## 6. DISCUSSION

The analysis for a one-carrier system, presented in the previous two sections, demonstrates that taking account of the deviation of the electron temperature from the lattice temperature, in a barrier region, leads to a voltage-current characteristic considerably different from the TEA value. Even the zero-bias resistance is appreciably altered unless the electron phonon coupling constant is (improbably) large. This is connected with the fact that $(T-1)$ is of order $j$, for small $j$, in the barrier region, as demonstrated in Sec. 4. However, in a uniform field region $(T-1)$ is of order $j^2$ [cf. Eq. (53) and subsequent remarks] so that the hot electron effect on the resistance disappears when $j$ tends to zero.

The results of the computation described in Sec. 5 were obtained on the assumption of electron scattering only by the acoustic modes of vibration. However, in materials where the frequency spectrum has an optical branch, the energy transfer from the electrons to the lattice is predominantly via optical phonons.[13] In that case, if the coupling constant $c$ refers to acoustic electron scattering only, the calculated difference between the electron temperature $T$ and the lattice temperature $T_0$ will be too large and the calculated voltage-current characteristic will deviate too much from the TEA solution. A very crude way of incorporating the effect of optical phonon scattering into the present calculation would be to take the velocity of sound larger than its true value thus increasing the coupling constant $c$ and enhancing the energy transfer. (In this connection it is of interest that Shockley[1] found reasonable agreement between the experimental mobility-field variation for

$n$-type Ge and theory, involving only acoustic scattering, for electron temperatures less than the optical mode temperature and a velocity of sound equal to 3.2 times the known value.)

As emphasized in Sec. 1, it would be entirely incorrect to incorporate the hot electron effect into barrier theory by using some field-dependent expressions for the mobility and diffusion constant in the expression for the current density [Eq. (1)]. Rather, using the assumption of a Maxwellian electron energy distribution, the dependence of the mobility and diffusion constant on electron temperature must be determined for the particular semiconductor under investigation. The electron temperature itself can only be determined for the particular structure being considered by solving the equation for conservation of energy simultaneously with the equation for the current density. Additional complications will arise for two carrier systems ($p$-$n$ junctions) where the carrier lifetimes which enter into the continuity equations are also carrier-temperature-dependent and electron and hole temperatures will in general be different.

Space-charge-limited current flow in dielectrics or $n-i-n$ structures is another one-carrier problem where the hot electron effect may be important. Dacey[31] has shown that the measured current in a $n-i-n$ Ge structure is in agreement with a theory which neglects the effect of diffusion and uses the observed dependence of mobility on field. The latter actually implies that the divergence of the energy flux $S$ in Eq. (7) can be neglected, as well as the diffusion term in Eq. (3), so that the electron temperature and consequently electron mobility are unique functions of the field and independent of the current. However, the inclusion of the diffusion term in the TEA has shown that there are regions of current where it is important.[32] Thus a complete solution for the hot electron effect on space-charge-limited currents requires the simultaneous solution of the three transport equations in Sec. 3 together with Poisson's equation.


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## APPENDIX

Terms involving $f_2(E,x)$ have been omitted in Eq. (13). These arise in the evaluation of the $P_1(\cos\theta)$, field and diffusion, terms and can only be neglected if

$$\frac{|f_1|}{\tau}\gg\frac{2}{5}\frac{p}{m^*}\left|\frac{\partial f_2}{\partial x}-eF\left(\frac{\partial f_2}{\partial E}+\frac{3}{2}\frac{f_2}{E}\right)\right| \tag{A1}$$

(unreduced variables will be used throughout the Appendix). The quantity $f_2(E,x)$ can be derived by solving for the $P_2(\cos\theta)$ terms of Eq. (11). This gives

$$\frac{2}{3}\frac{eFp}{m^*}\left(\frac{\partial f_1}{\partial E}-\frac{f_1}{E}\right)-\frac{2}{3}\frac{p}{m^*}\frac{\partial f_1}{\partial x}-\frac{f_2}{\tau_2}=0, \tag{A2}$$

neglecting terms involving $f_3(E,x)$. The relaxation time $\tau_2$ can be derived from Eq. (A7) in the first reference 10 taking $f_2(E\pm\epsilon)$ approximately equal to $f_2(E)$. For the particular case of acoustic scattering,

$$\tau=lm^*/p,\quad \tau_2=(3/7)lm^*/p, \tag{A3}$$

where $l$ is the mean free path, independent of the electron energy $E$.

The condition (A1) can now be evaluated by substituting for $f_0$, $f_1$, and $f_2$ from Eqs. (20), (13), and (A2), respectively. This leads to a very complicated result involving various products of higher order derivatives of $F$, $n$, and $T$, with respect to $x$. As an approximation, consider first that terms involving the field $F$ are predominant while diffusion terms (involving differentiation with respect to $x$) can be neglected. Then, using Eqs. (A2) and (A3), condition (A1) becomes

$$\frac{5}{2}\frac{|f_1|}{l}\gg\frac{2}{7}e^2F^2l\left|\frac{\partial}{\partial E}\left(\frac{\partial f_1}{\partial E}-\frac{f_1}{2E}\right)+\frac{3}{2E}\left(\frac{\partial f_1}{\partial E}-\frac{f_1}{2E}\right)\right|. \tag{A4}$$

Since $f_1(E)$ is proportional to $\exp(-E/kT)$, condition (A4) will be satisfied, for arbitrary $E$ of order $kT$, when

$$eFl\ll kT, \tag{A5}$$

dropping numerical factors of order one. This is the only condition[33] usually stated for the TEA (cf. reference 19) where $T$ is equal to $T_0$.

Consider next that the diffusion terms are predominant while the field terms may be neglected. Then condition (A1) becomes

$$\frac{5}{2}\frac{|f_1|}{l}\gg\frac{2}{7}l\left|\frac{\partial^2 f_1}{\partial x^2}\right|. \tag{A6}$$

From Eqs. (13) and (20) (neglecting the term due to $F$),

$$f_1=-l\left[\frac{d(\ln n)}{dx}+\left(\frac{E}{kT}-\frac{3}{2}\right)\frac{d(\ln T)}{dx}\right]f_0, \tag{A7}$$

where the first term corresponds to ordinary diffusion and the second to thermal diffusion. Substituting into (A6), it will be found that if ordinary diffusion is predominant, then the condition

$$l^2|d^3n/dx^3|\ll|dn/dx| \tag{A8}$$

[31] G. C. Dacey, Phys. Rev. 90, 759 (1953).
[32] W. Shockley and R. C. Prim, Phys. Rev. 90, 753 (1953).
[33] In the TEA one can easily eliminate $f_2$ between inequality (A1) and Eq. (A2) without considering field and diffusion terms separately. It turns out that inequality (A1) will then be satisfied if $el^2dF/dx\ll kT_0$ in addition to inequality (A5).

must be satisfied; if thermal diffusion is predominant,

$$\frac{l d(\ln T)}{dx}, \quad \frac{l^2 d^2(\ln T)}{dx^2}, \quad \frac{l^2 d^3(\ln T)/dx^3}{d(\ln T)/dx} \ll 1 \qquad \text{(A9)}$$

must be satisfied.

To test whether terms containing $f_2(E,x)$ can be neglected in a particular case, it is necessary to evaluate the various derivatives in inequalities (A5), (A8), and (A9) from the computed solutions and see if the inequalities are satisfied. For scattering mechanisms with an energy-dependent mean free path, the conditions will remain essentially unaltered with $l$ evaluated for the average electron energy $kT$.

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# Theory of Superconductivity. I. Electron-Lattice Interaction

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The electron-lattice interaction responsible for electrical resistivity in perfect metallic crystals is shown to be a form of Jahn-Teller effect. It does not occur in the Born-Oppenheimer (adiabatic) approximation even when the electron-electron interaction is taken fully into account. The matrix elements that describe corrections to the Born-Oppenheimer approximation are derived by a general argument that can be applied to metals with arbitrary electronic energy band structure, and the case of monatomic metals is worked out in detail in the effective mass approximation. Two types of physical phenomena are attributed to these matrix elements. The first is ordinary electrical resistivity due to electron-phonon scattering. The present derivation leads to the same formal structure as the usual theory, but should give quantitatively different results when applied to specific metals. The second type of physical phenomenon is a modification to the stationary states of the electron-lattice system that can significantly alter the total energy spectrum at low energies, and mixes states of electron excitation and lattice excitation. An effect of this kind can account qualitatively for the disappearance of electrical resistivity at finite temperatures in superconductors. Other special properties of superconductors should follow from consideration of the stationary states modified by the Jahn-Teller effect.

## I. INTRODUCTION

THE theory of superconductivity[1] developed by Bardeen, Cooper, and Schrieffer and by Bogoliubov successfully accounts for the thermodynamic behavior of superconductors at low temperatures, the dependence of critical temperature on isotopic mass, and other properties dependent upon the existence and magnitude of an energy gap for electron excitations. However, the Meissner effect (expulsion of the magnetic field) follows from an argument that has been the subject of considerable controversy[2] and cannot be said to be an immediate intuitive result of the theory. The phenomenon of superconductivity itself (vanishing resistivity at a finite temperature) is not explained by the theory.[2] The theory is based on a highly simplified form of the Hamiltonian, which, although representing the most important terms in the complete Hamiltonian, leaves out most of the structure both of the phonon frequency spectrum and of the electronic energy bands.

It has been pointed out by several authors[3] that the electron-lattice interaction must be thought of as a correction to the Born-Oppenheimer or adiabatic approximation, and that this must affect the theory of superconductivity. Matrix elements for transitions described as electron-phonon scattering are unchanged to first order from those of the Bloch theory.[3] However, matrix elements also occur between nondegenerate Born-Oppenheimer states. The present paper will derive these matrix elements in more detail than did the authors cited, in order to establish a basis for discussion of the stationary (or metastable) states of the interacting electron-lattice system. This leads to a reformulation of the theory of superconductivity that includes a more realistic description of the phonon energy spectrum and the electronic band structure than is possible in the Bardeen-Cooper-Schrieffer theory. Since the field-theoretical formalism does not lend itself to a detailed discussion of the degeneracies that occur, which are qualitatively very important in treating the electron-phonon interaction, the present analysis will be carried out in terms of the Schrödinger wave functions of the system.

The exact nonrelativistic Hamiltonian for a metal

[1] J. Bardeen, L. N. Cooper, and J. R. Schrieffer, Phys. Rev. **108**, 1175 (1957); N. N. Bogoliubov, Nuovo cimento (10) **7**, 794 (1958); J. Exptl. Theoret. Phys. (U.S.S.R.) **34**, 58 (1958); N. N. Bogoliubov, V. V. Tolmachev, and D. V. Shirkov, *A New Method in the Theory of Superconductivity* (Academy of Sciences of U.S.S.R., Moscow, 1958).

[2] M. R. Schafroth, in *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic Press Inc., New York, 1960), Vol. 10, pp. 293–498.

[3] J. M. Ziman, Proc. Cambridge Phil. Soc. **51**, 707 (1955); H. Stumpf, Z. Naturforschung **11a**, 259 (1956); A. Haug, Z. Physik **146**, 75 (1956); B. Goodman, Phys. Rev. **110**, 888 (1958).