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Electron Tunneling in Metal-Semiconductor Barriers

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Tunneling through the space-charge region of a uniformly doped semiconductor has been calculated in the effective-mass approximation. The exact solutions of the one-dimensional Schrödinger equation for a parabolic potential are used to determine the transparency of the barrier. Numerical results are presented for parameters appropriate to indium and *n*-type germanium. An example of experimental results typical of this system is quoted to illustrate qualitative agreement.

I. INTRODUCTION

IN this paper we present a calculation for the dependence of tunneling current on applied voltage bias in metal-semiconductor junctions. Alternatively, this can be regarded as a calculation of the departure from ideal behavior in a type of noninjecting Ohmic contact. Tunneling in the rectifying metal-semiconductor contact, which is more popularly known as the Schottky barrier diode, was considered earlier, but not in detail. A discussion of the earlier calculations and of the Schottky model, which we adopt, is presented by Henisch.[1] More recently, Padovani and Stratton[2] have analyzed tunneling in the Schottky barrier from the standpoint of thermionic-field emission.[3] Other closely related calculations are those of Esaki,[4] Keldysh,[5,6] and Kane[7,8] on tunneling in *p*-*n* junctions. However, they have not considered the dependence of electron transmission on energy and applied bias which prove to be essential features in the metal-semiconductor tunneling. Shuey[9] has calculated formal expressions for direct tunneling with improvements in this respect. His results, however, are not directly applicable.

To obtain an expression for the tunneling current, we generalize a result (29) of Fredkin and Wannier.[10]

$$j=-2e\int \frac{d^3\mathbf{k}_l}{(2\pi)^3} v_{rz}|T_{l\to r}|^2[\mathfrak{F}(E_l)-\mathfrak{F}(E_r)]. \quad (1)$$

In this form, $\mathbf{k}_r$ has been related to $\mathbf{k}_l$ by assuming conservation of transverse momentum and energy, i.e., $\mathbf{k}_{\perp l}=\mathbf{k}_{\perp r}$ and $E_r=E_l-eV_a$. The barrier transparency $|T_{l\to r}|^2$ is obtained through the solution of a Schrödinger equation. Since we assume uniform impurity density n_r in the semiconductor, the barrier potential is essentially parabolic and an exact solution is obtained.

In Sec. II we present the model, discuss the most significant simplifications, and obtain an expression for the dependence of the potential barrier on applied bias. An expression for the barrier transparency $|T_{l\to r}|^2$ appropriate to this potential is derived in Sec. III. Particulars regarding evaluation of the tunneling integral (1) are presented in Sec. IV along with numerical results for parameters pertaining to the system of indium and *n*-type germanium. An example of experimental results from this materials system are quoted in Sec. V to illustrate the existence of a qualitative agreement. These results are presented in terms of the dependence of incremental resistance $(dj/dV)^{-1}$ on applied bias. A significant feature of this characteristic is a maximum which is shown to occur at an applied bias V_a which corresponds to the Fermi degeneracy μ_r of the semiconductor.

The results derived apply strictly to a semiconductor which is appropriately described by a single conduction band, centered in reciprocal space and of spherical symmetry. An extension of this result to more general types of band structure, e.g., many-valley, is important. Done explicitly, relatively complicated expressions are obtained. Results from the more elementary model, however, can be used without loss of significance and an entirely satisfactory quantitative approximation can be made through an argument detailed in Sec. VI.

II. THE METAL-SEMICONDUCTOR BARRIER

The idealized potential energy diagram of Schottky for a semiconductor in contact with a metal is shown in Figs. 1(a)-(c) for zero, forward, and reverse biases, respectively. The semiconductor as represented is *n*-type, uniformly doped, and degenerate. The states occupied at $T=0$°K are indicated. At the energy of minimum barrier width, $d_{\min}$, arrows are drawn in the direction of electron tunneling. This width is larger at zero bias than for either sign of applied bias. This is responsible for the tunneling characteristics of present interest and causes a considerable departure from the rectification with which the Schottky barrier is usually associated.

The dependence of the potential $\varphi(z)$ in the depletion

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[2] F. A. Padovani and R. Stratton, Bull. Am. Phys. Soc. **11**, 239 (1966).

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[9] R. T. Shuey, Phys. Rev. **137**, A1268 (1965).

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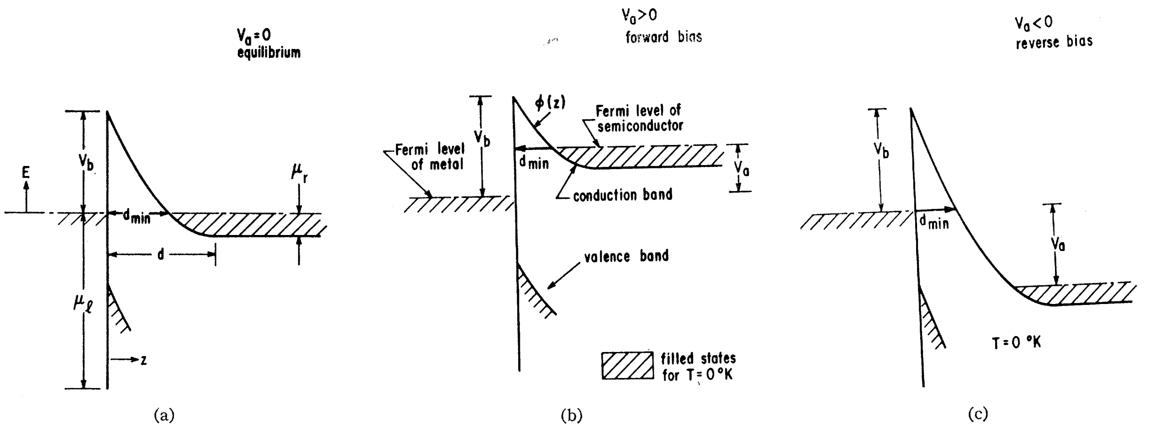

FIG. 1. Idealized potential energy diagrams for a metal-semiconductor interface in the cases of (a) zero bias, (b) forward bias, (c) reverse bias. Note that the minimum distance $d_{\min}$ through which an electron tunnels is maximum at zero bias.

layer of a semiconductor of uniform impurity density n_r is essentially parabolic,

$$\varphi(z)=e^2n_r(d-z)^2/2\epsilon_r+e(V_a-\mu_r) \quad 0<z<d. \tag{2}$$

This is obtained as a solution of a simplified Poisson's equation, and departs from the exact solution in the reserve region $d_{\min}<z<d$. This difference is most significant where the tunneling distance is largest, and hence, of least concern. The effect of the image charge is also neglected. For the particular problem of interest, the difference, which is practically independent of applied bias, is small and produces no significant effect on the results. Energy in Eq. (2) and subsequent expressions is measured with respect to the Fermi surface of the metal.

As indicated in Fig. 1, the potential $\varphi(z)$ is locked to the interface to a value $\varphi(0)=eV_b$ which is independent of doping and bias. This condition determines the width and bias dependence of the depletion layer,

$$d=[2\epsilon_r(V_b+\mu_r-V_a)/en_r]^{1/2}. \tag{3}$$

Electrons in the metal are characterized by a spherical energy surface of Fermi degeneracy μ_l, density n_l, and effective mass m_l which is assumed to equal the free mass m_0. Similarly, electrons in the semiconductor are described by μ_r, n_r, and m_r.

III. BARRIER TRANSPARENCY

Consider an electron flux impinging upon the junction from the left. A fraction R_l is reflected and a fraction $T_{l\to r}$ is transmitted. The wave functions describing this are obtained by solving a Schrödinger equation for each of these regions and applying the appropriate joining conditions. The appropriate Hamiltonian written in terms of the barrier potential (2) is

$$\begin{aligned} H &= -\frac{\hbar^2}{2m_l}\frac{d^2}{dz^2}, && z<0; \\ &= -\frac{\hbar^2}{2m_r}\frac{d^2}{dz^2}+\varphi(z), && 0<z<d; \\ &= -\frac{\hbar^2}{2m_r}\frac{d^2}{dz^2}+e(V_\alpha-\mu_r), && z>d. \end{aligned} \tag{4}$$

The wave function obtained is

$$\begin{aligned} \Psi &= I_0\{\exp(ik_{lz}z)+R_l\exp(ik_{lz})\}, && z<0; \\ &= I_0\{A\mathfrak{U}(-\kappa_{rz}^2,\zeta)+B\mathfrak{V}(-\kappa_{rz}^2,\zeta)\}, && 0<z<d; \\ &= I_0\{T_{l\to r}\exp[ik_{rz}(z-d)]\}, && z>d; \end{aligned} \tag{5}$$

where $\mathfrak{U}$ and $\mathfrak{V}$ are parabolic cylinder functions[11] and

$$\lambda^4\equiv \hbar^2\epsilon_r/4m_re^2n_r, \tag{6a}$$

$$\kappa_{rz}\equiv\lambda k_{rz}, \tag{6b}$$

$$\zeta\equiv(d-z)/\lambda. \tag{6c}$$

The wave functions for the three regions must be matched at the two boundaries. The proper matching conditions are that $\Psi(z)$ and $m(z)^{-1}d\Psi(z)/dz$ be continuous. The latter condition assures time-reversal invariance and continuity of current.

In applying the effective-mass formalism, we assume that $\varphi(z)$ does not change appreciably in a lattice spacing. Further, we assume that the value of effective mass m_r appropriate to allowed states properly describes the tunneling electron.

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[11] J. C. P. Miller, in *Handbook of Mathematical Functions*, edited by M. Abramowitz and I. A. Stegun (U. S. Department of Commerce, National Bureau of Standards, Washington, D. C., 1964), Appl. Math. Ser. 55, p. 685.

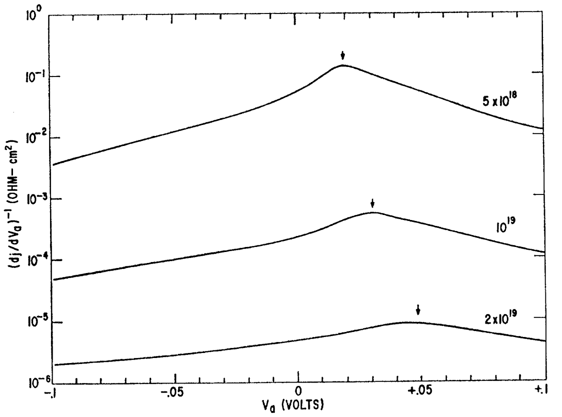

FIG. 2. Incremental resistance, plotted versus applied bias, for indium on degenerate *n*-type germanium. The resistance is maximum for biases equal to the Fermi energy of the germanium electrons, whose Fermi energy is indicated by an arrow (↓). This calculation is described in Secs. III and IV, and the parameters used are listed in Table I.

The transmission obtained by the matching procedure is

$$\begin{aligned}T_{l\to r}=2(2/\pi)^{1/2}\{&[\mathfrak{U}(-\kappa_{rz}^2,\zeta_0)+i\mathfrak{U}'(-\kappa_{rz}^2,\zeta_0)/\kappa_{lz}]\\&\times[i\kappa_{rz}\mathfrak{V}(-\kappa_{rz}^2,0)+\mathfrak{V}'(-\kappa_{rz}^2,0)]\\&-[\mathfrak{V}(-\kappa_{rz}^2,\zeta_0)+i\mathfrak{V}'(-\kappa_{rz}^2,\zeta_0)/\kappa_{lz}]\\&\times[i\kappa_{rz}\mathfrak{U}(-\kappa_{rz}^2,0)+\mathfrak{U}'(-\kappa_{rz}^2,0)]\}^{-1},\end{aligned}\tag{7}$$

where

$$\zeta_0\equiv d/\lambda,\tag{8a}$$

$$\kappa_{lz}\equiv\lambda k_{lz}m_r/m_l,\tag{8b}$$

$$\mathfrak{U}'(-\kappa_{rz}^2,\zeta_0)=\partial\mathfrak{U}(-\kappa_{rz}^2,\zeta)/\partial\zeta|_{\zeta_0}\text{ etc.}\tag{8c}$$

In evaluating (7), the functions at $\zeta=0$ are known, and those at ζ_0 are found by asymptotic expansion[11] for $\zeta_0\gg|-\kappa_{rz}^2|$. In this approximation, the barrier transparency is

$$|T_{l\to r}|^2=\frac{4}{\pi}\frac{(\frac{1}{2}\zeta_0^2)^{\kappa_{rz}^2+\frac{1}{2}}}{[1+(\frac{1}{2}\zeta_0\kappa_{lz})^2]}\times\frac{\exp(-\frac{1}{2}\zeta_0^2)}{[\Gamma^{-2}(\frac{1}{4}-\frac{1}{2}\kappa_{rz}^2)+(\frac{1}{2}\kappa_{rz}^2)\Gamma^{-2}(\frac{3}{4}-\frac{1}{2}\kappa_{rz}^2)]}.\tag{9}$$

IV. TUNNELING CHARACTERISTICS

To facilitate evaluation, the tunneling integral (1) is rewritten in the form

$$j=-eg_{lf}v_{lf}\int_{-\infty}^{\infty}dE[\mathfrak{F}_l(E)-\mathfrak{F}_r(E-eV_a)]\times\int_0^{\nu_{\max}}\nu d\nu\frac{\kappa_{rz}}{\kappa_{lr}}|T_{l\to r}|^2.\tag{10}$$

For the spherical system of coordinates used, $\nu\equiv\sin\theta$ and θ is the angle between $\mathbf{k}_l$ and the current, z, axis. Since the applied bias voltage V_a is generally much smaller than the Fermi degeneracy of the metal μ_l, the density of states g_{lf} and Fermi velocity v_{lf} are treated as constants. Conservation of the transverse components of momentum and of energy requires

$$\hbar^2k_{rz}^2/2m_r=E+e(\mu_r-V_a)-(E+e\mu_l)\nu^2m_l/m_r,\tag{11a}$$

and

$$k_{lz}=k_{lf}(1-\nu^2)^{1/2}.\tag{11b}$$

The integrations over energy E and angle ν are limited to the range where k_{rz} is positive and real.

The tunneling current as a function of applied bias and temperature can readily be obtained from (9) and (10) by numerical means. However, a particularly useful result is formed when the tunneling characteristic is plotted in terms of incremental resistance $(dj/dV_a)^{-1}$. An example of this is shown in Fig. 2, where characteristics are shown for several values of impurity density. For each curve, a maximum occurs at an applied bias which corresponds to the Fermi degeneracy of the semiconductor. (The small arrow shown denotes this value.) The sign of applied bias at the maxima is as shown in Fig. 1(b).

Parameters used in the numerical evaluation are listed in Table I and are appropriate to the sysetm of indium and *n*-type germanium. The Fermi degeneracy of the metal μ_l was calculated in the free-electron approximation. The barrier V_b height shown is $\frac{2}{3}$ of the

TABLE I. Parameters employed in evaluating (9) and (10) for the case of indium and *n*-type germanium.

Parameter	Value taken
m_l	m_0
m_r	$0.12m_0$
V_b	0.52 eV
μ_l	8.6 eV
ϵ_r	$16\epsilon_0$
T	0°K

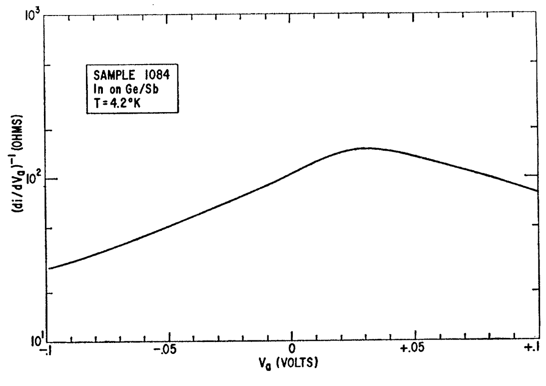

FIG. 3. A selected experimental example of the tunneling characteristic of In and *n*-type germanium (to be compared with the dependence in Fig. 2 corresponding to $n_r=1\times10^{19}$ cm^{-3}).

energy gap as measured near 0°K.[12,13] The degeneracy in the semiconductor μ_r is related to impurity concentration through a published value of the density of states effective mass.[14] Carrier "freeze-out" is assumed not to occur.

V. AN EXPERIMENTAL RESULT

As an example of experimental results, the characteristics of a sample made by alloying indium to n-type germanium is shown in Fig. 3. The Fermi degeneracy $\zeta_r = 0.031$ eV and impurity concentration $N_d = 1.0 \times 10^{19}$ were estimated on the basis of a resistivity measurement. The general features compare favorably with the theoretical dependence shown in Fig. 2. We elect, however, to defer a discussion of this particular result as well as the more general aspects of our experiments.[15]

VI. CONCLUDING DISCUSSION

The derivation presented applies strictly to a semiconductor with zone-centered conduction band of spherical symmetry. This is readily generalized to include the case of a valence band. The significant difference in results from the two cases is a reversal in the dependence with respect to the sign of applied bias. If the structure shows degeneracy, the band of lightest mass is most significant. The many-valley structure forms another important case. A detailed solution for this has been made. The results obtained from this are essentially equivalent to the results from the elementary model and need not be presented. The underlying reasons for this can be demonstrated by means of a simple physical argument.

Two features of the many-valley problem are significant. The surfaces of constant energy are described as ellipsoids and they are not centered in reciprocal space. One implication of this is the requirement that the effective mass be taken as the component of the tensor along the axis of the tunneling current. For an axis of sufficient symmetry, all ellipsoids may be equivalent in this respect. Further, the displacement of the centers of the ellipsoids is generally smaller than the radius of the Fermi sphere of a metal. Hence, momentum $\mathbf{k}_\perp$ can be conserved directly, i.e., without phonon assistance. This effects a marked difference between tunneling in metal-semiconductor and p-n junctions. Details in the integration differ from those of the spherical and zone-centered situation but only with respect to geometry. In practice these details do not make any significant difference.

For these reasons, results based on the derivation presented, properly weighed for the number of valleys and the component of tensor mass in the tunneling direction, can be expected to be in excellent qualitative agreement and retain all the physical significance of the more involved situations. In the particular case of Ge, there are four equivalent minima on $\langle 111 \rangle$ axes of masses $m_{\parallel}/m_0 = 1.6$ and $m_\perp/m_0 = 0.0819$ which are centered at the edge of the reduced zone.[16] For a tunneling current axis in the $\langle 100 \rangle$ direction they are equivalent and have $m_r = 0.12$ as a mass component. This is the value listed in Table I on which the results shown in Fig. 2 are based.

We have calculated the tunneling characteristic of metal-semiconductor junctions and have obtained qualitative results in a form which is suited to direct comparison with experiment. One application of particular importance is the noninjecting Ohmic contact of device technology. Such a comparison, however, should most properly be considered to be qualitative. To do more would require a degree of accuracy in specification of the parameters which is not in general available. A maximum in the incremental resistance is predicted at a bias potential which corresponds to the Fermi degeneracy of the semiconductor. This offers a technique for the direct observation and quantitative measurement of degeneracy.

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[12] C. A. Mead and W. G. Spitzer, Phys. Rev. **134**, A713 (1964).

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[15] J. W. Conley and J. J. Tiemann (to be published).

[16] For a survey of the literature regarding this see R. A. Smith, *Semiconductors* (Cambridge University Press, New York, 1959), Chap. 10.