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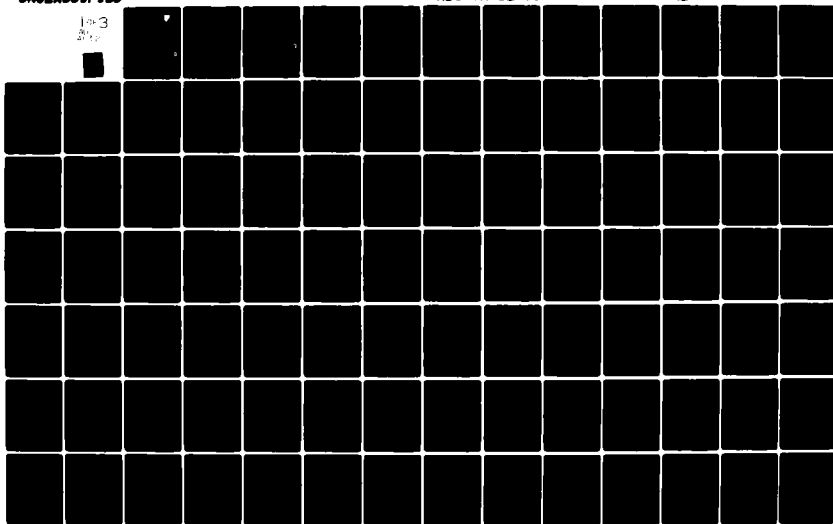
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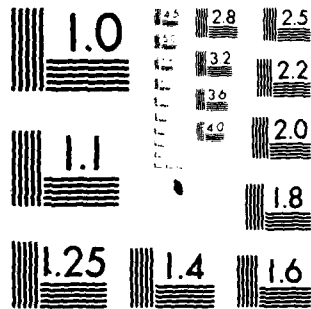
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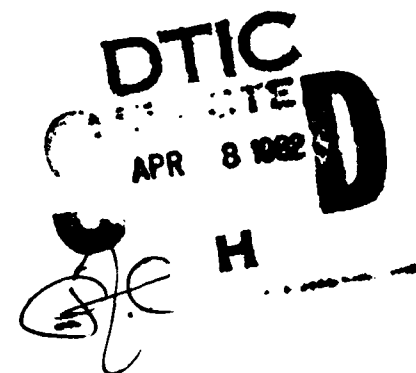


INVESTIGATION OF THE CURRENT VOLTAGE RELATIONSHIP FOR LOW BARRIER SCHOTTKY DIODES

D. P. Kennedy & Associates, Inc.

David P. Kennedy

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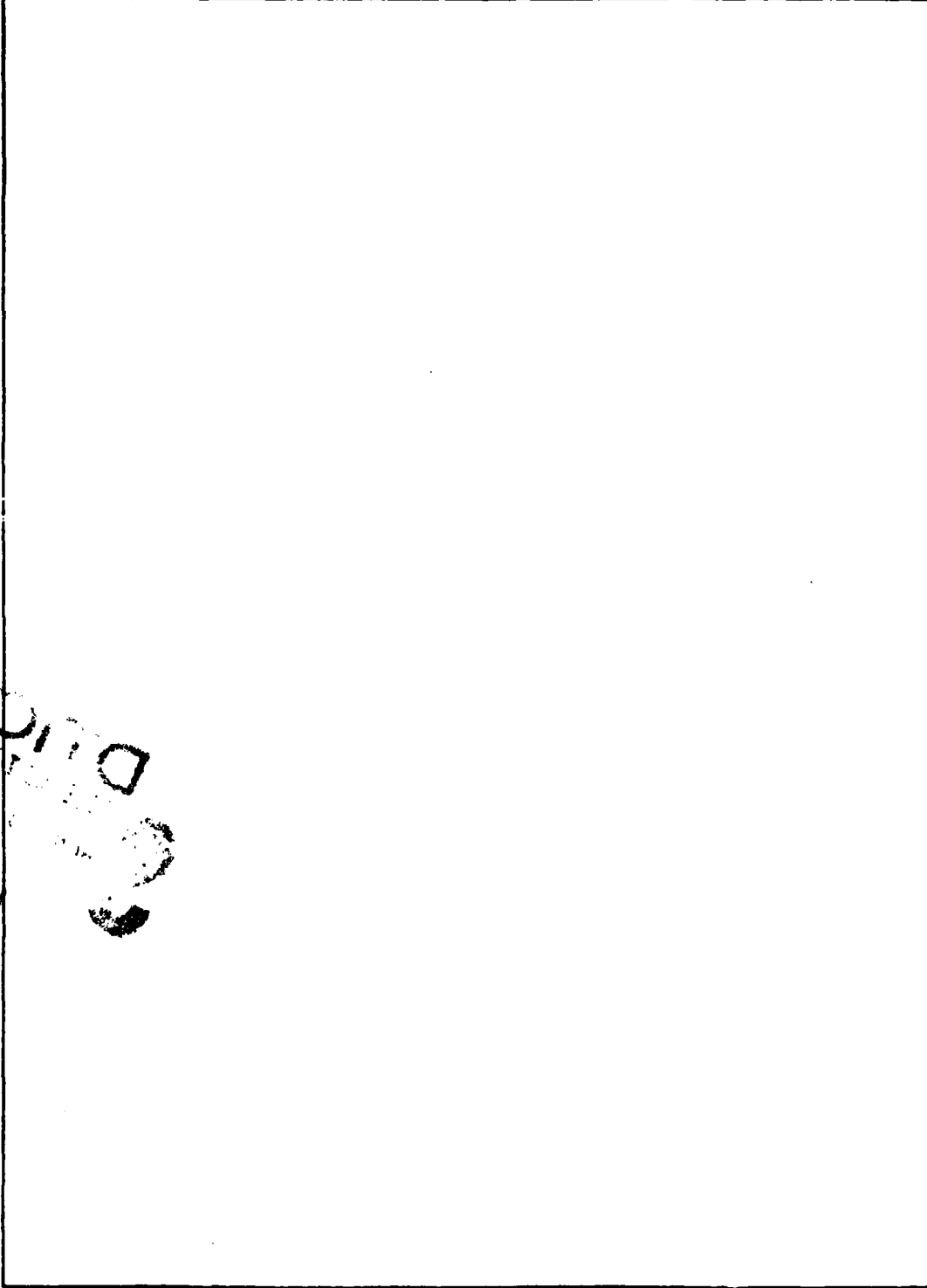
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Statement of Work

Under Contract No. 19628-80-C-0020 D.P. Kennedy & Assoc., Inc. has undertaken investigations into the current-voltage relationship of low barrier Schottky diodes. A particular objective of this program was to develop understanding of the large reverse current observed in Pt-Si diodes on p-type silicon, when operating at low temperatures (77° to 110° K). Additionally, after identification of appropriate physical mechanisms it was desired to undertake rigorous numerical investigations of the topic. Such numerical investigations could offer a means for quantitative comparisons between theory and measurements upon experimental Pt-Si semiconductor devices.

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Summary and Major Results

The topic of this investigation was based upon experimental observations of an exceedingly large reverse electric current, as exhibited by p-type Pt-Si Schottky barrier diodes when operating at a low ambient temperature (77° - 110° K). Numerous explanations of this phenomenon are based upon a proposed mechanism of hole generation within metallurgical regions of this device. It has been suggested that such holes transverse the interface barrier, much like conduction electrons in an n-type Schottky barrier diode and, thereafter, produce the observed electric current. Because hole generation, in the classical sense, cannot exist in a metallic conductor, this investigation was directed toward other mechanisms; mechanisms capable of producing a large reverse electric current.

Calculations show that an insignificant number of mobile electrons exist in p-type silicon at low ambient temperatures (77° to 110° K) and, therefore, the observed reverse electric current is unlikely to arise from normal hole/electron pair generation within the silicon space-charge layer. As a consequence, the observed electric current is suggested to arise from mobile hole generation at the silicon-metal interface through mechanisms heretofore given little recognition in the technical literature. Specifically, it is proposed that silicon valence electrons enter unoccupied electron states within the metallic conductor and, thereby, produce mobile holes without a traditional hole-electron pair generation in the semiconductor material.

A study of the technical literature was undertaken on the topic of electron field-emission from silicon. Some experimental data on electron field emission has been interpreted as arising from electron emission from the valence band of p-type silicon. Additionally, using approximation methods other workers have shown that field emission from the valence band should, indeed, be expected from p-type silicon.

It is important to note that these studies of field-emission from silicon were undertaken with no apparent recognition of applicable mechanisms for p-type Schottky barrier diodes.

From traditional theory of metallic conductors, it is shown that a large number of unoccupied energy states exist below the Fermi-level. Additionally, it is shown that interface valence electrons can enter these unoccupied states with a degree of excitation below that required by classical theory for this type of electron transition. As a consequence, an effective energy barrier could be defined for a p-type Schottky barrier that is less than that given by traditional theory of metal-semiconductor contacts.

For a p-type Schottky barrier, detailed calculations are presented for the reverse electric current. These calculations are based upon traditional concepts drawn from the statistical theory of matter. Specifically, the rate is calculated at which electron transitions take place from the semiconductor valence band to the conduction band of the metallic contact. Such calculations have been undertaken for a large assumed range of conduction band free electron density; a range that would include both degenerate semiconductor material and an ideal metal.

Resulting from these calculations is much understanding about the mechanisms involved in the operation of a p-type Schottky barrier. It is demonstrated that despite the experimental observation of bidirectional electric current, a true interface energy barrier exists in only a limited type of p-type semiconductor device. In particular a small reverse electric current can arise from one, or both, of two different mechanisms. A small reverse current can arise from the distribution of unoccupied energy states in the metal conduction band, relative to the energy band structure of the p-type semiconductor material. Additionally, an energy barrier in the classical sense can be shown when the conduction band edge of the metal is at a higher energy than the valence band edge of the semiconductor. This second mechanism will probably exist only if the adjacent

material is a highly degenerate semiconductor, rather than a metal. In line with the basic objectives of this research, many calculations were undertaken on the expected reverse current from low barrier semiconductor devices---defining the interface energy barrier in a manner consistent with current textbook concepts. It is shown that relatively poor rectification characteristics should exist for low barrier devices, if the contacting material is a true metal. If, instead, the contacting material is a degenerate n-type semiconductor the rectification properties could be substantially improved, although in most cases the expected reverse current will be larger than calculated from classical concepts of Schottky barrier operation.

For a rigorous study of this topic a computer program was developed that is capable of calculating the electrostatic potential in a reverse biased Schottky barrier diode, in the presence of a large electric current. This computer program involves the simultaneous solution of Poisson's equation and the mobile hole continuity equation. Two distinctly different hole generation mechanisms are utilized: first, the classical HSR hole-electron generation through a single mid-gap recombination center and, second, hole generation from the top of the valence band. This computer program is capable of accurately calculating the Schottky barrier potential distribution, even in the presence of a large reverse electric current. Insufficient time was available during the present contract period to complete coupling this rigorous solution to the calculation of electron transition at the metal/semiconductor interface.

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Chapter I

Theory of Operation for a p-type Schottky Barrier

1.0 Introduction

Experiment shows that low-barrier Schottky barrier diodes on p-type silicon exhibit poor rectification qualities, even at low ambient temperatures. Such experiments have directed workers toward a rigorous study of physical mechanisms associated with this type of semiconductor device. In particular, the physical mechanisms contributing to a large reverse electric current. Therein we have the basis and direction of the present research on Schottky barrier operation. A principle goal for this research is to undertake a mathematical study of the physics associated with the poor reverse current characteristics of the Schottky barrier diode, placing particular emphasis upon devices composed of Pt-Si on p-type silicon.

An initial survey of the technical literature shows that most theory of Schottky barrier diode operation is based upon devices containing n-type semiconductor material. This theory is in detail and mathematically rigorous. Furthermore, comparisons between theory and experiment are in qualitative agreement, and many are in quantitative agreement, for most of the important characteristics exhibited by this device. A source of difficulty in such comparisons has always been a lack of detailed knowledge about the structure of the metal-semiconductor interface. Theoretical investigations are frequently based upon an idealization of this interface, an idealization that renders the problem tractable from a mathematical and physical point of view.

Nonetheless, it is believed safe to say that an extensive understanding is available on the operation of n-type metal-semiconductor contacts of the rectifying and non-rectifying types. Clearly, because of the similarity between n-type and p-type metal-semiconductor contacts it has been a great temptation to explain p-type device operation using the theory for n-type devices---with, of course, suitable modifications. A particularly difficult extension of this n-type device theory has been the need to explain the reverse current in p-type Schottky barriers, when operating at a low ambient temperature. At low temperatures the hole-electron pair generation is insufficient to explain the large reverse electric current exhibited by this semiconductor diode.

In reverse biased n-type Schottky barrier a nearly unlimited supply of mobile electrons reside within the metallic contact. If, indeed, within this source some electrons have sufficient energy to overcome the interface potential barrier, these electrons will contribute to the reverse electric current. Contrasting with this n-type device concept, no such obvious supply of mobile carriers exists for the p-type Schottky barrier. It is evident that the reverse electric current in a p-type device arises from holes moving from the depletion layer to charge neutral regions of the semiconductor. An important question is the source of these holes, particularly at an ambient temperature that decreases generation/recombination to a negligible value.

It has been a generally accepted practice to assume hole generation within the metallic contact of a p-type Schottky barrier and, thereby, imply a substantial degree of similarity between n-type and p-type device operation. If, indeed, holes were generated in the metal, the theory of p-type diode operation would be a simple extension of n-type device theory. It must be acknowledged that mobile holes, as such, cannot exist within a metallic conductor and, therefore, the theory of p-type Schottky barrier operation is in great difficulty.

There is little question that the reverse electric current must arise from mobile holes within the space-charge region of a p-type device. Additionally, it must be acknowledged that these mobile holes do not arise from hole-electron pair generation alone. If generation/recombination mechanisms represented the only source of mobile holes, we could not explain the large magnitude of reverse current at low device temperatures. Instead, new mechanisms of hole generation must be proposed; mechanisms whereby mobile holes are generated without necessarily generating conduction band electrons.

The basis of the present research is to investigate a new mechanism of the foregoing type. Specifically, it is proposed that hole generation can exist at the metal-semiconductor interface by valence electron transitions from the semiconductor to unoccupied states within the metallic conductor. Further, it is suggested that through this mechanism we can explain the low temperature reverse electric current characteristics exhibited by low-barrier Schottky devices on p-type silicon. Additionally it is suggested that this mechanism will often render such a physical structure electrically Ohmic at room temperature.

2.0 Field Emission from Semiconductor Materials

For many years electron emission from electrical conductors has been a topic of extensive investigation. There are two basic mechanisms whereby this emission can take place: first, at high temperatures (Thermionic emission) and, second, when a conductor is exposed to a large electric field in a direction normal to its surface (Field emission). At high temperatures free electrons within a conductor acquire sufficient energy to overcome an electrostatic potential barrier present at its surface. At large values of normally directed electric field the surface barrier of a material can become exceedingly thin and, thereby, permit tunneling from the material to free space.

Emission experiments using semiconducting material have brought renewed interest to this subject. In particular, two distinctly different field-emission characteristics can be demonstrated for n-type and p-type silicon and germanium [1-4]. Further, some experiments show that n-type silicon can exhibit the field emission properties of n-type or p-type silicon. These two distinctly different emission characteristics have been explained theoretically [5]; the first type is proposed to result from the emission of valence band electrons.

It is emphasized that these studies were directed toward the topic of field-emission, with no reference to implications associated with device theory. Nonetheless, field-emission from the valence band represents hole generation without the generation of an associated conduction band electron. If, indeed, these field-emission workers demonstrate valence band emission from silicon, there is little reason to neglect this mechanism in the theory of Schottky barrier diode operation.

3.0 Unoccupied Energy States in a Metallic Conductor

In the present discussion we focus upon the density and distribution of unoccupied energy states in a conductor that reside between the Fermi-level E_f and the conduction band edge E_c . It will be shown that a significant quantity of these unoccupied states are far removed from the Fermi-level, and there is no reason to assume $E_f - E_b$ in Fig. 1 represents a real energy barrier in a p-type Schottky device. In particular many silicon valence electrons at the metal-semiconductor interface that undergo thermal excitation can, indeed, enter the metal at an energy substantially below the traditionally assumed Fermi-level.

The distribution of unoccupied energy states is particularly dependent upon the position of the Fermi-level, relative to the conduction band edge. Additionally, this Fermi-level is temperature dependent; we must first establish its magnitude, as a function of temperature. This

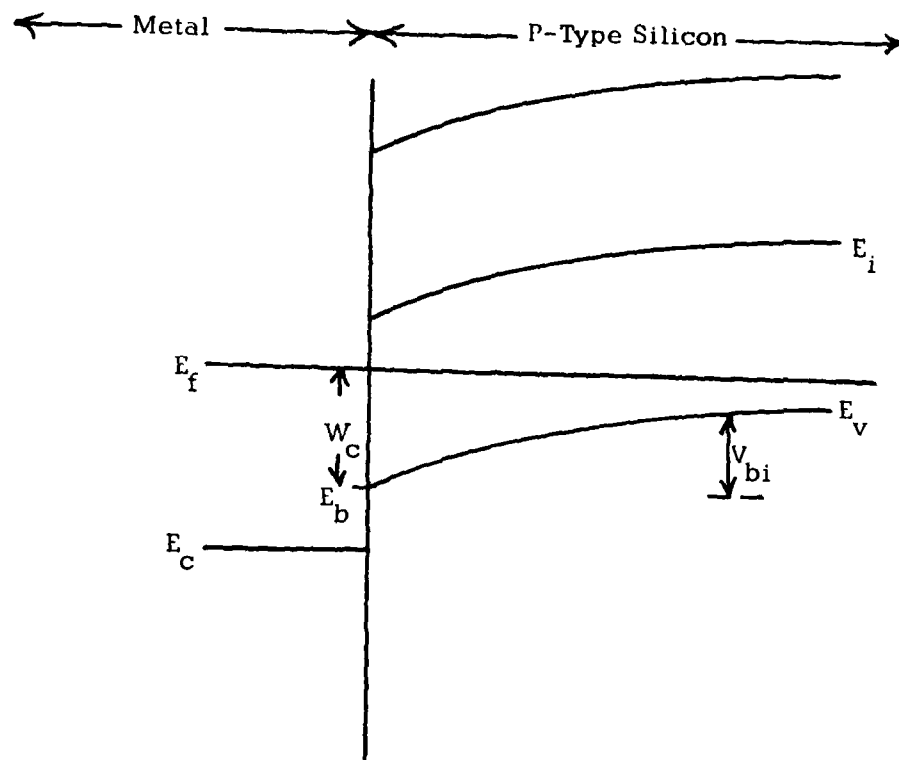


Fig.1 Energy Band Diagram for a Schottky Barrier on P-Type Silicon

is easily accomplished using the conventional density of states equation [6],

$$\Delta N = 8\pi\sqrt{2}(\sqrt{m}/h)^3\sqrt{E} \Delta E \quad (1-1)$$

in combination with the Fermi-Dirac distribution

$$P(E) = \left[1 + \exp (E - E_f) / kT \right]^{-1} . \quad (1-2)$$

Upon combining Eq.(1-1) and Eq.(1-2) we have the familiar density of occupied energy states that reside between E and (E + ΔE),

$$\Delta N = 8\pi\sqrt{2}(\sqrt{m}/h)^3\sqrt{E} \left[1 + \exp (E - E_f) / kT \right]^{-1} \Delta E \quad (1-3)$$

clearly, the total density of these occupied states in a metal is given by

$$N_c = 8\pi\sqrt{2}(\sqrt{m}/h)^3 \int_0^{\infty} \frac{\sqrt{E} dE}{1 + \exp (E - E_f) / kT} \quad (1-4)$$

Equation (1-4) has been used to calculate the Fermi-level in a metal as a function of temperature. We first assume in Eq.(1-4) that T = 0 yielding

$$N_c = 8\pi\sqrt{2}(\sqrt{m}/h)^3 \left[\frac{2}{3} E_{f0}^{3/2} \right] \quad (1-5)$$

where N_c is the density of conduction electrons and E_{f0} is the Fermi energy at T = 0. Thereafter, we combine Eq.(1-4) and Eq.(1-5) and solve for E_f

$$1 = \frac{3}{2} E_{f0}^{-3/2} \int_0^{\infty} \frac{\sqrt{E} dE}{1 + \exp (E - E_f) / kT} . \quad (1-6)$$

Figure 2 illustrates this Fermi-level calculation assuming a density of states effective mass of unity. Clearly, calculating the Fermi-level is an iterative process and must be accomplished through numerical integration techniques; the computer program used for this calculation is listed in APPENDIX IA. In all calculations presented in this report the forementioned computer program was used for calculating the Fermi-level.

Only a minor modification of Eq.(1-4) is required to calculate the density of unoccupied energy states that reside between the Fermi-level and the conduction band edge,

$$N = 8\pi \sqrt{2} (\sqrt{m}/h)^3 \int_{E_c}^{E_f} \frac{\sqrt{E} dE}{1 + \exp (E - E_f) / kT} . \quad (1-7)$$

Figure 3 illustrates this calculation throughout a wide temperature range, and throughout a range of free electron density frequently encountered in a metallic conductor.

From Fig.3, at 77° K conductors with a free electron density within the range $10^{20} \leq N_c \leq 10^{23}$ can be expected to contain about 10^{18} to 10^{19} unoccupied energy states between the Fermi-level and the conduction band edge. Clearly, this is a non-negligible quantity if we wish to assume $E_f - E_b$ in Fig.1 represents an energy barrier that limits the reverse electric current in a Schottky diode.

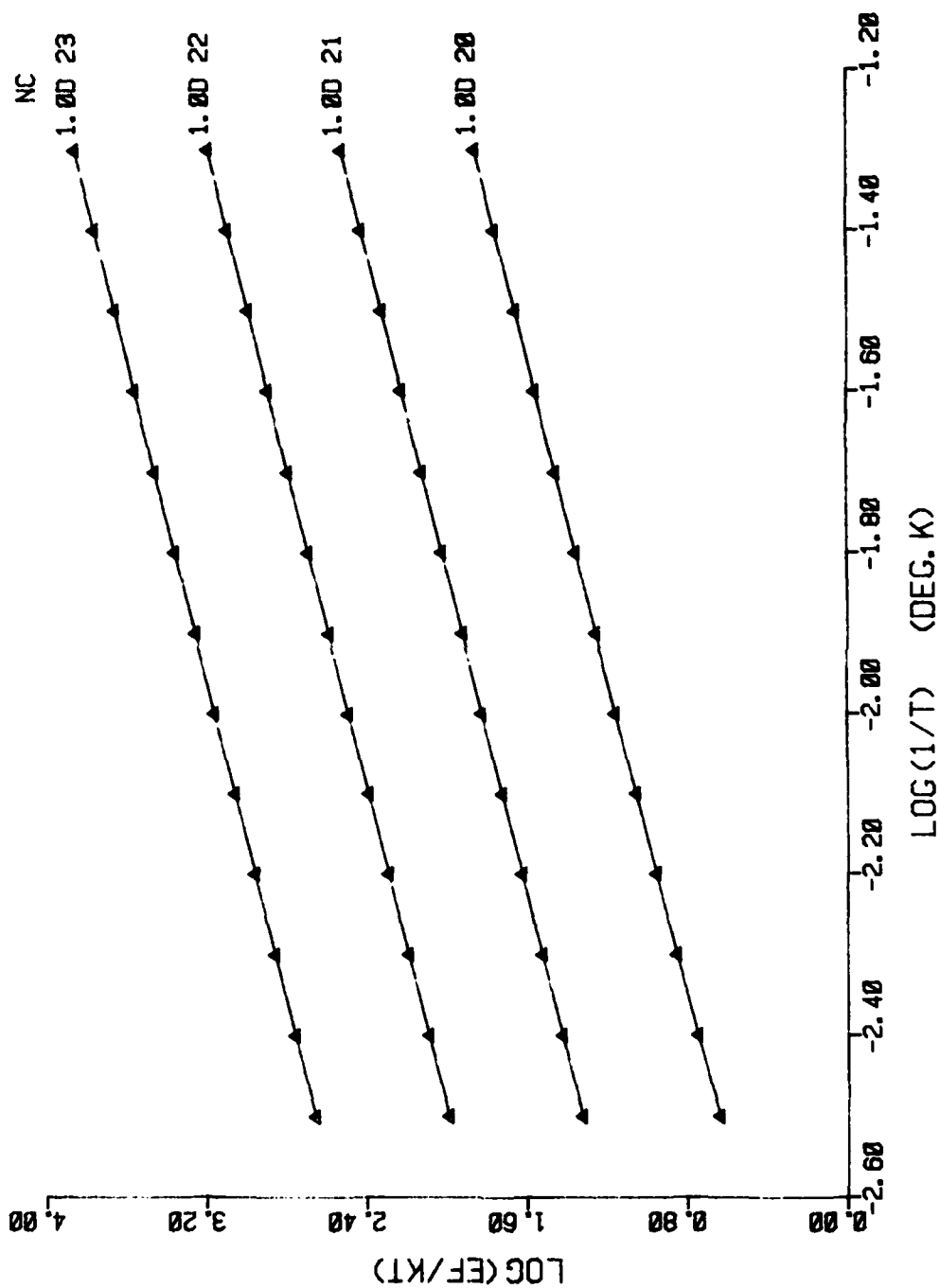


Fig. 2 Fermi Level in a Metal Containing a Free Electron Density of N_C

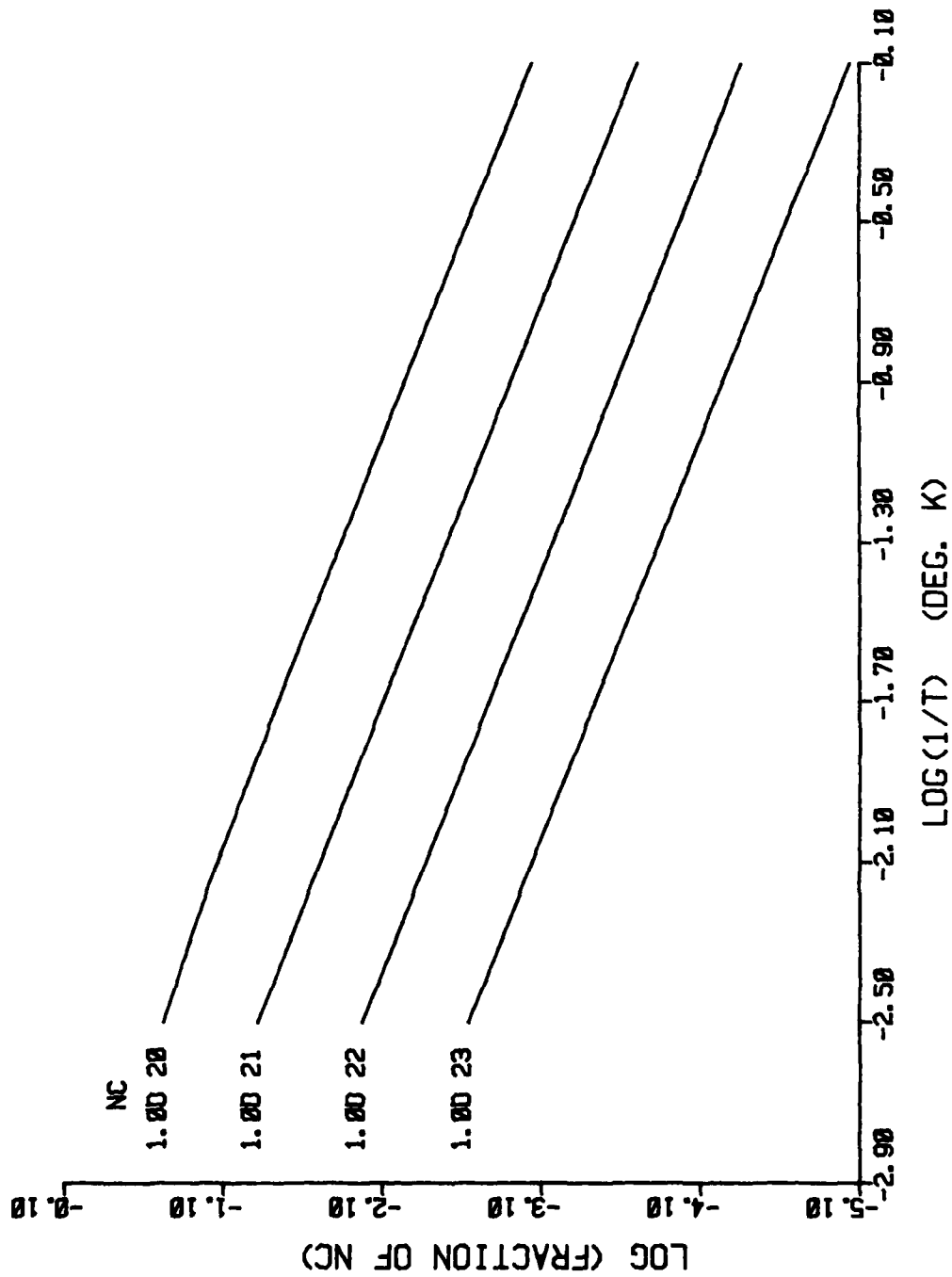


Fig. 3 Density of Unoccupied Energy States in a Metal Between the Conduction Band Edge E_c and the Fermi-Level. N_c = Free Electron Density

An equally important aspect of this concept is the distribution of these unoccupied energy states within the range $E_c \leq E \leq E_f$. Clearly, if the majority of these unoccupied states are clustered near the Fermi-level we could retain the concept of a potential barrier of $E_f - E_b$ in a Schottky diode. If, instead, a large quantity of states reside near the energy E_b in Fig.1, we must reconsider the concept of reverse electric current in this semiconductor device.

Again, by numerically integrating the expression

$$N = 8\pi\sqrt{2} (\sqrt{m}/h)^3 \int_{E_b}^{E_f} \frac{\sqrt{E}}{1 + \exp(E - E_f)/kT} dE \quad (1-8)$$

We evaluate the quantity of unoccupied states that reside throughout the energy range $E_b \leq E \leq E_f$. Such calculations are presented in Fig. 4 through Fig. 6 for a range of assumed locations for E_b .

This sequence of calculations clearly show that the density of unoccupied states are, indeed, clustered near the Fermi-level. For example, material containing a free electron density of $10^{22} \text{ (cm}^{-3}\text{)}$, Fig.(6), exhibit a negligible difference in vacant state density between $E_b/E_f = 0.1$ and $E_b/E_f = 0.98$, at a temperature of 77°K . Similarly, at room temperature material with a free electron density of $10^{21} \text{ (cm}^{-3}\text{)}$, Fig.5, exhibits an unoccupied energy state density of about $1.25 \times 10^{19} \text{ (cm}^{-3}\text{)}$ within 2% of the range $(E_f - E_b)$ from the Fermi-level. Nonetheless, it is recognized that in a Schottky diode the remaining unoccupied energy states could produce a significant magnitude of reverse current.

A further amplification of this topic is obtained by numerically integrating Eq.(1-4) throughout the range $E_c \leq E \leq E_b$,

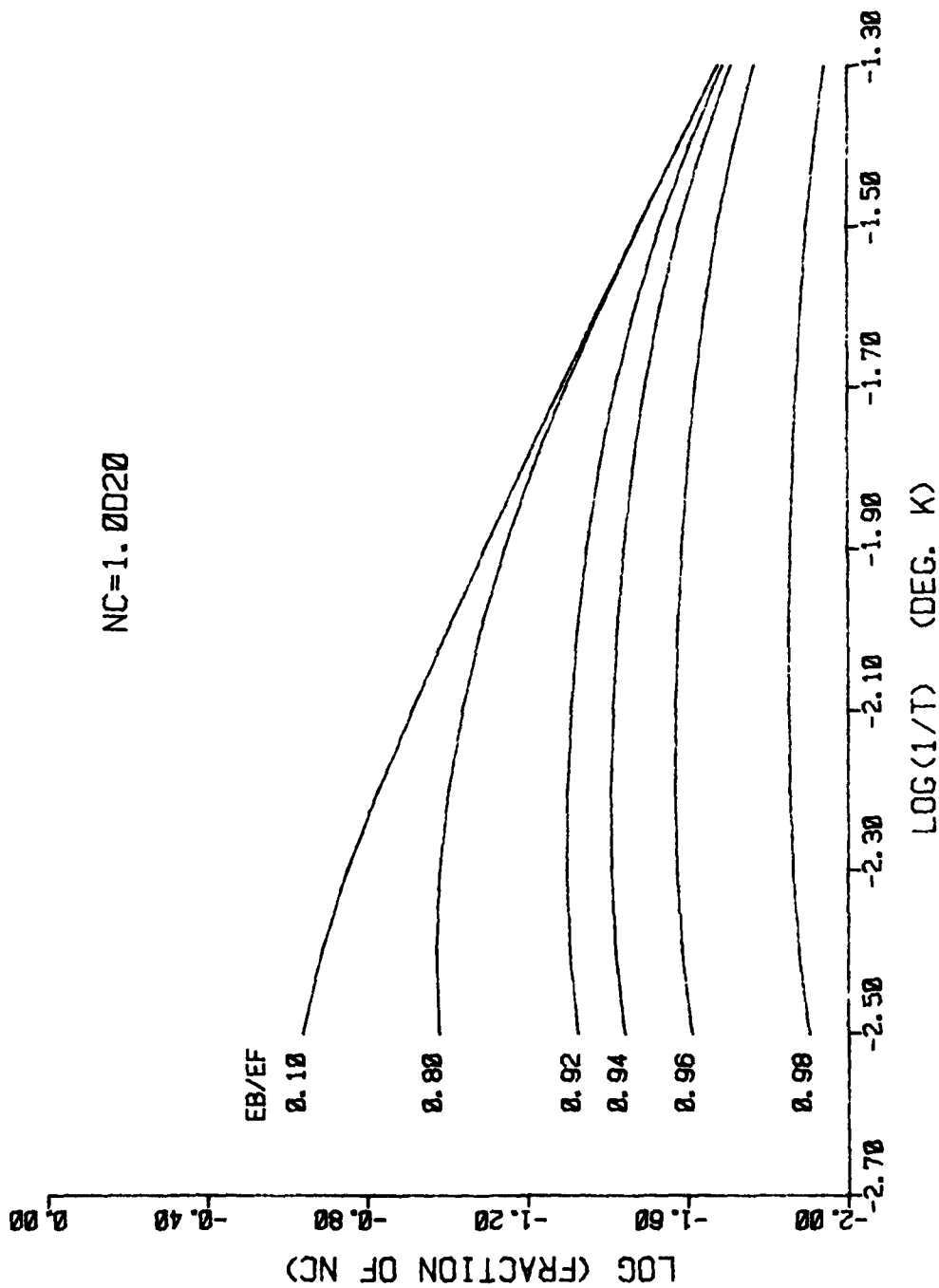


Fig. 4 Density of Unoccupied Energy States Between the Fermi-Level, E_f and an Energy E_b where $E_c < E_b < E_f$

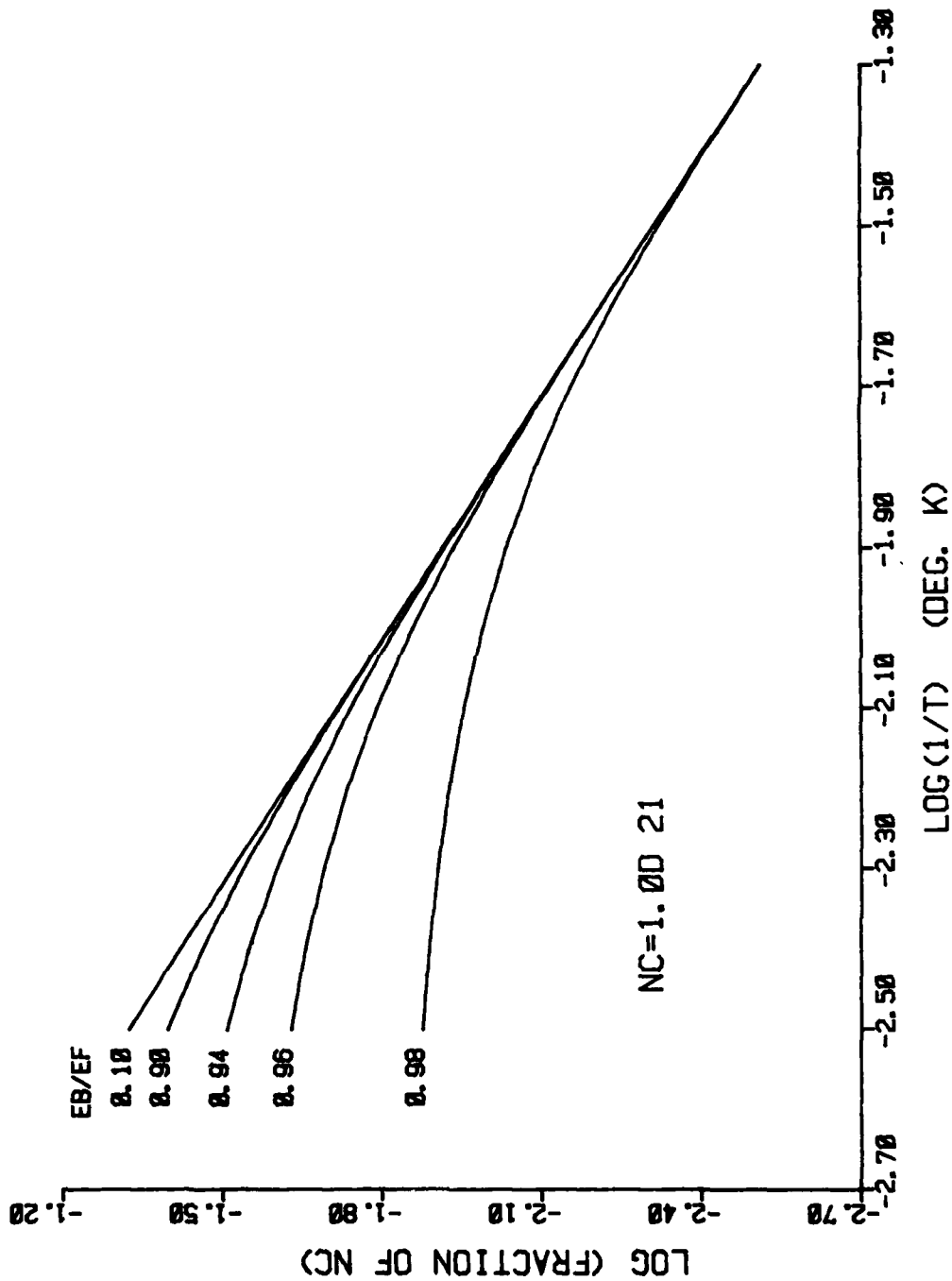


Fig. 5 Density of Unoccupied Energy States Between the Fermi-Level and an Energy E_b where $E_c < E_b < E_f$

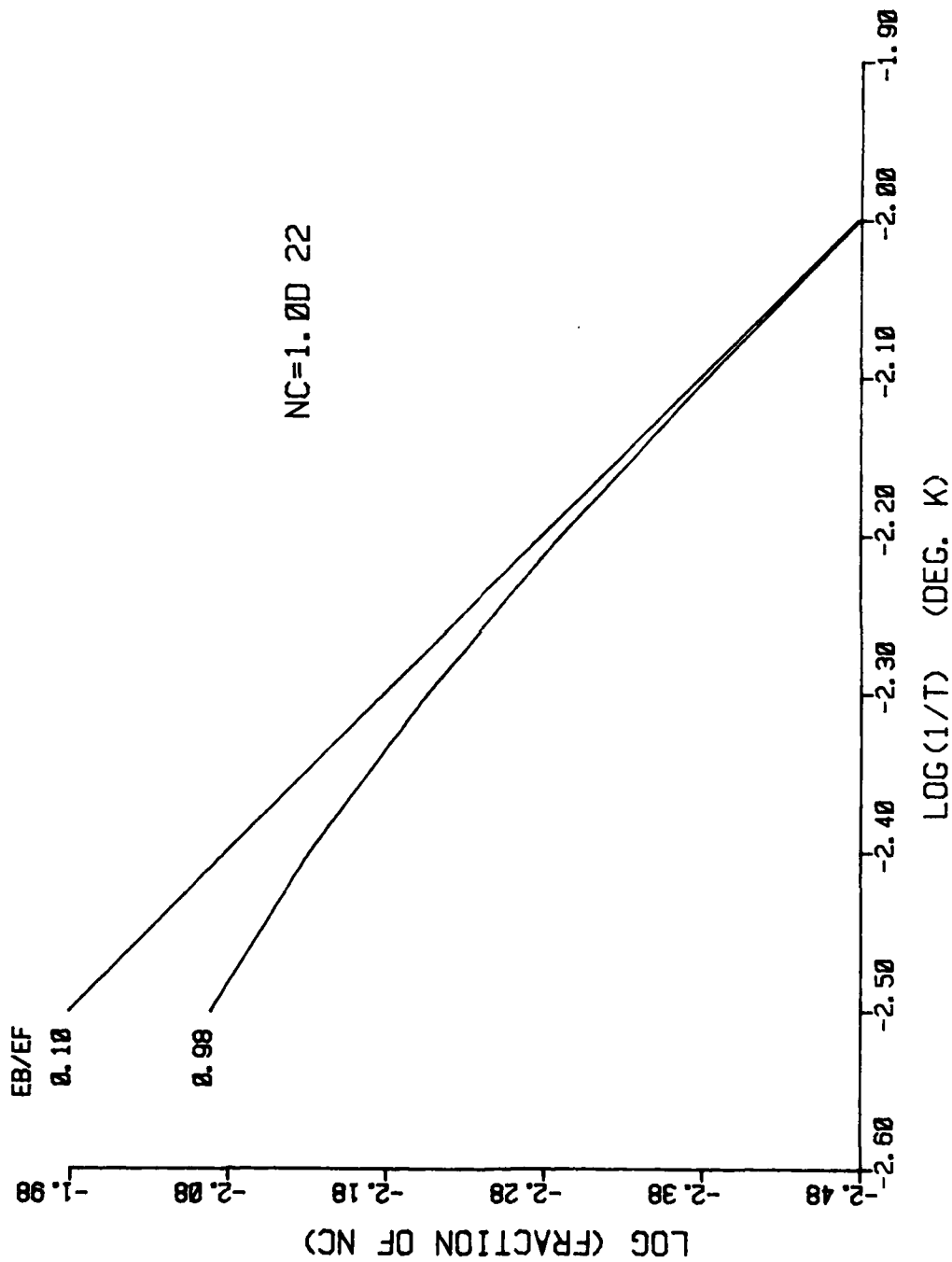


Fig. 6 Density of Unoccupied Energy States Between the Fermi Level E_f and an Energy E_b where $E_b < E_f$

$$N = 8\pi\sqrt{2} (\sqrt{m}/h)^3 \int_{E_c}^{E_b} \frac{\sqrt{E} dE}{1 + \exp (E_f - E_c) / kT} . \quad (1-9)$$

This calculation yields the density of unoccupied states that reside in the lower energy regions of the conduction band.

Figure 7 through Fig.10 illustrate this calculation throughout a range of free electron density of $10^{20} \leq N_c \leq 10^{23}$. These calculations clearly show that material containing a larger free electron density have the smallest density of unoccupied states in the lower regions of the conduction band. For example, at 77° K a free electron density of $10^{20} \text{ (cm}^{-3}\text{)}$, Fig.7, exhibits about $10^{14} \text{ (cm}^{-3}\text{)}$ unoccupied states in the lower 50% between E_f and E_c . At this same temperature material containing a free electron density of $10^{22} \text{ (cm}^{-3}\text{)}$ contain approximately $10^8 \text{ (cm}^{-3}\text{)}$ unoccupied states in the lower 92% of the energy between E_f and E_c .

The reason for this foregoing situation is attributable to the increase of $(E_f - E_c)$ with free electron density, Fig.2. An increase of $E_f - E_c$ produces a decrease of probability that the lower energy electrons can be excited to an energy level above E_f .

In the following sections of this report the computer programs used for calculations thus far illustrated are an integral part of all calculations directed toward the operation of Schottky barrier devices.

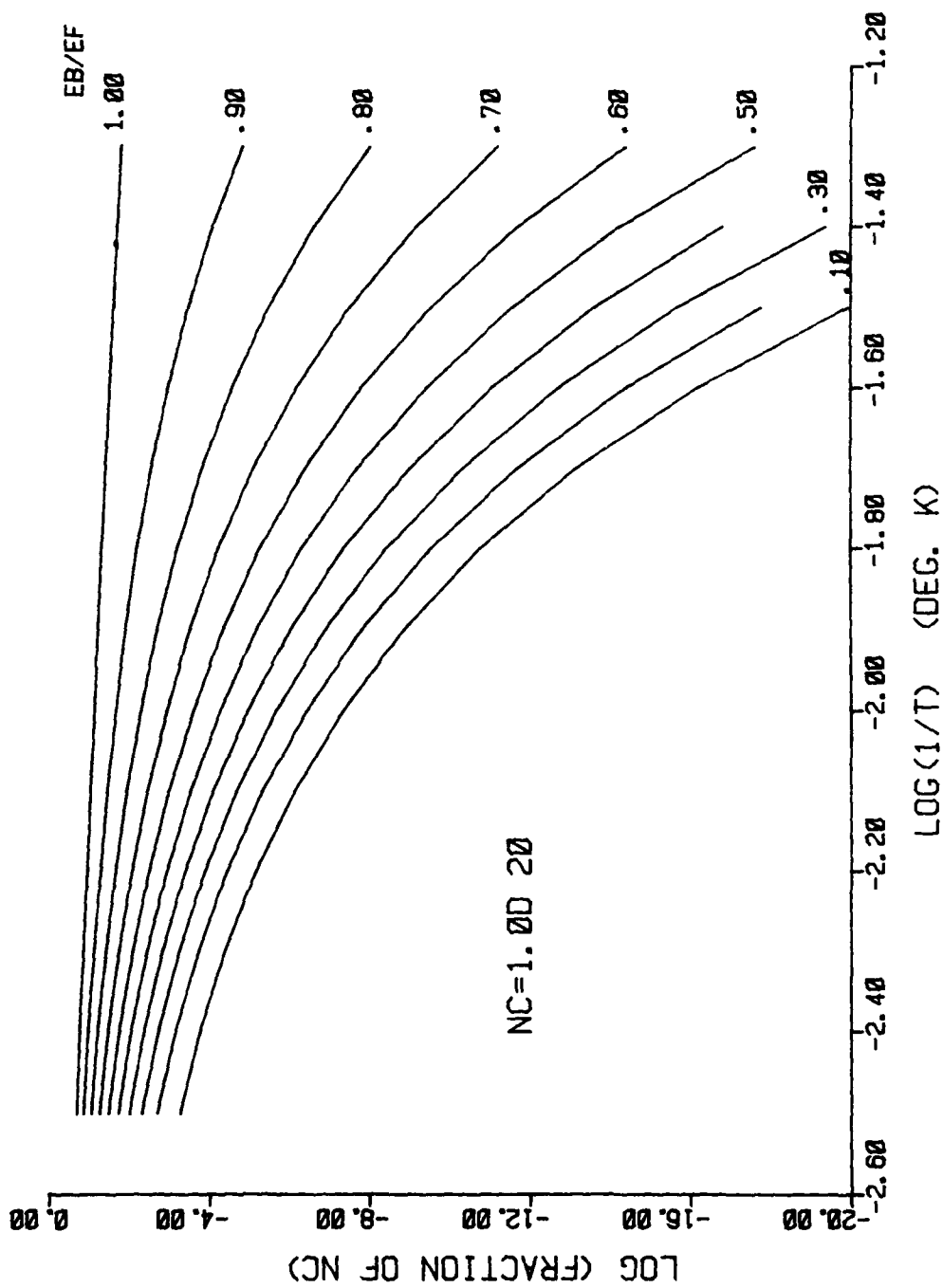


Fig. 7 Density of Unoccupied Energy States Between the Conduction Band Edge E_C and an Energy E_b where $E_C < E_b < E_f$

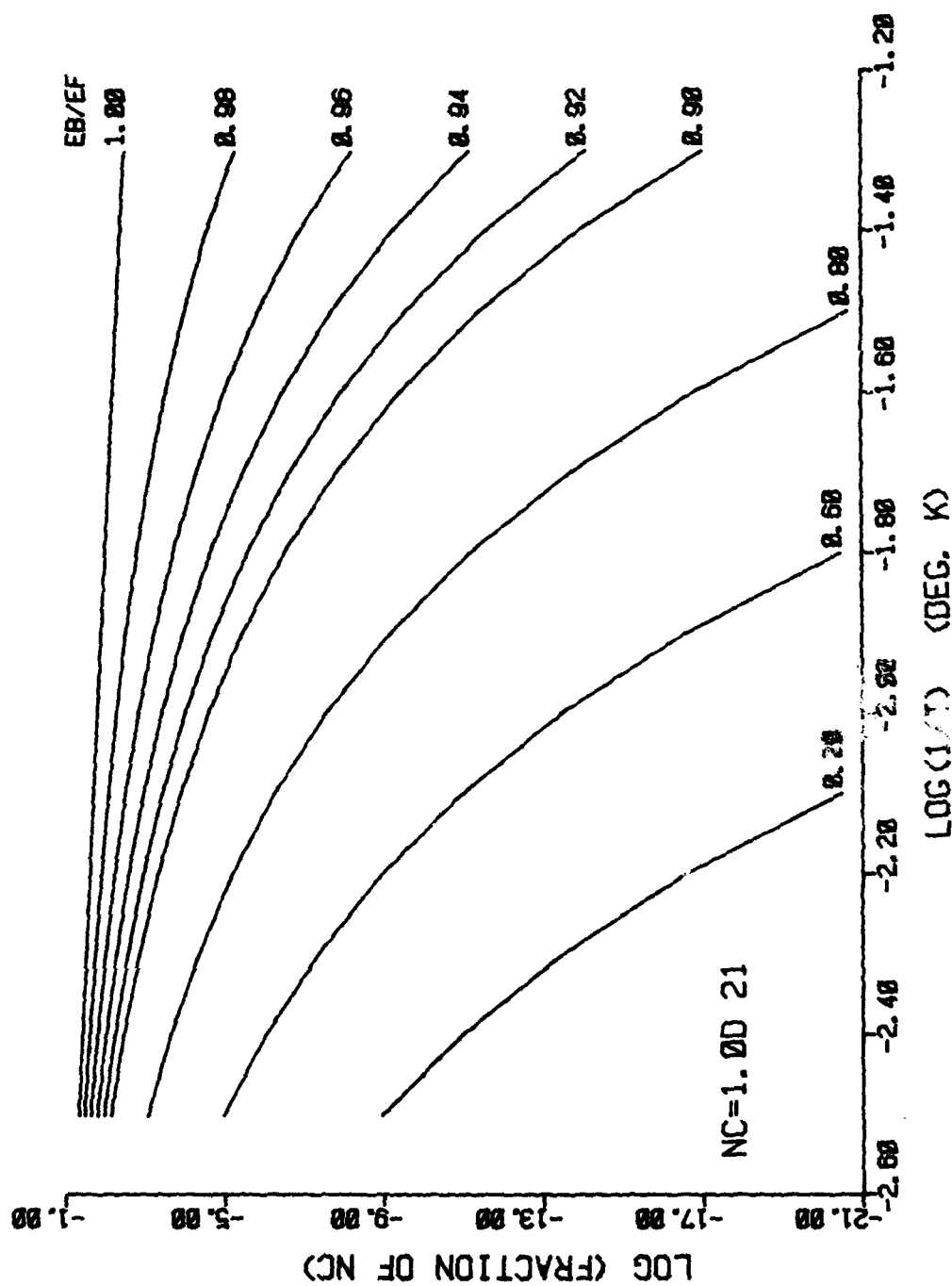


Fig. 8 Density of Unoccupied Energy States Between the Conduction Band Edge and an Energy E_b where $E_b < E_f$

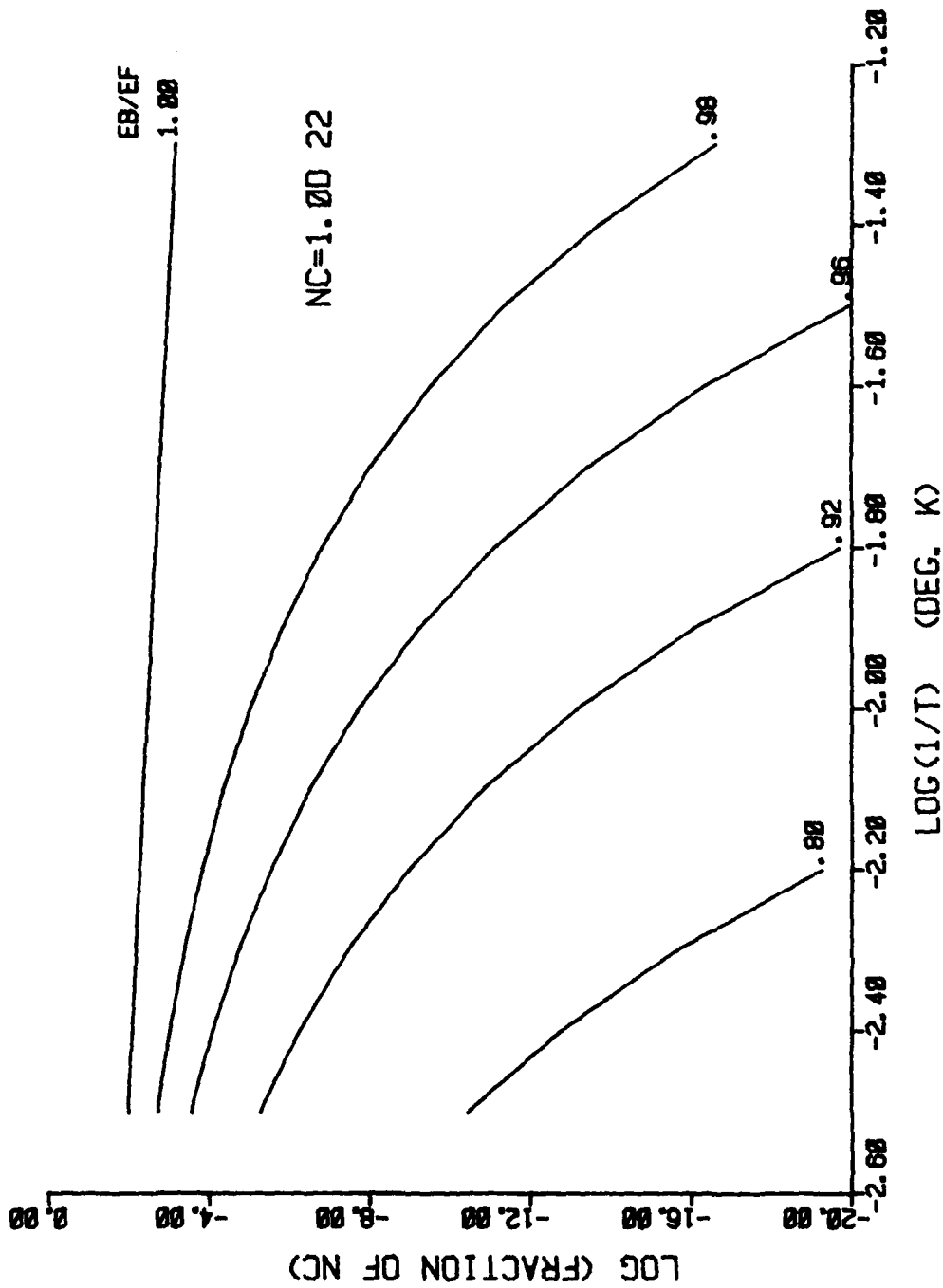


Fig. 9 Density of Unoccupied Energy States Between the Conduction Band Edge and an Energy E_b where $E_c < E_b < E_f$

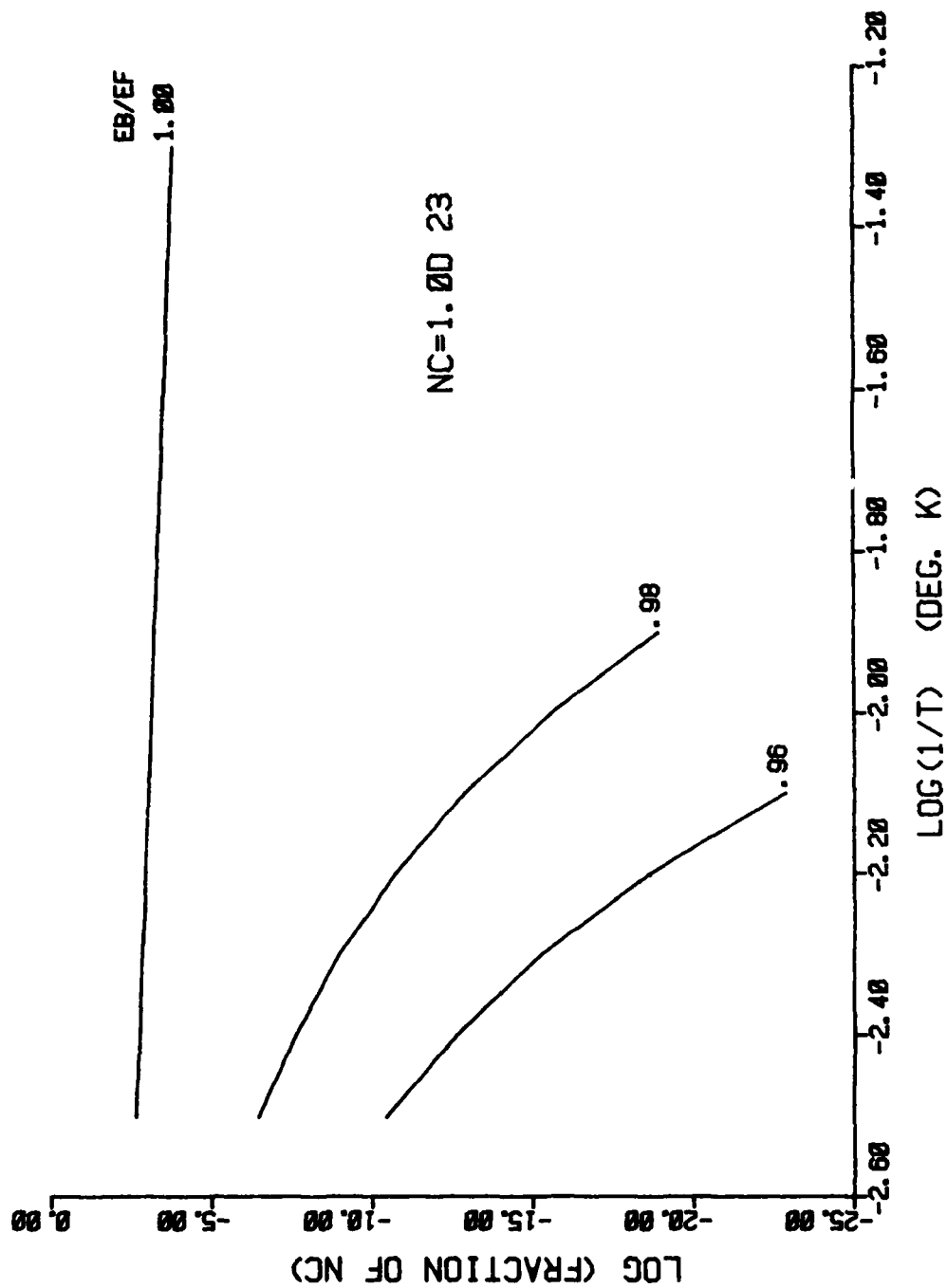


Fig.10 Density of Unoccupied Energy States Between the Conduction Band Edge E_C and an Energy E_b where $E_C < E_b < E_f$

4.0 The Transition Energy in a Schottky Barrier

In the conduction band of a metal the density of unoccupied energy states between E and $(E + \Delta E)$ is given by

$$\Delta N = 8\pi\sqrt{2} (\sqrt{m}/h)^3 \sqrt{E} \left[1 + \exp(E_f - E)/kT \right]^{-1} \Delta E . \quad (1-10)$$

If, indeed, semiconductor valence band electrons are to enter this conduction band there must be a place for them to go. If the number of electrons attempting to enter this conduction band at an energy E exceed the density of unoccupied states, many could return and not contribute to the electric current. If, instead, the density of unoccupied states at an energy E exceeds the source of supply, all valence band electrons attempting to enter the metal conduction band will find a place to go, and will contribute to the barrier electric current.

Next we consider the density of semiconductor valence band electrons that are attempting to enter this metallic conduction band. From Fig.1, all valence band electrons at an energy in excess of E_b must have undergone thermal excitation. Because all energy eigenvalues of the wave equation become imaginary in the forbidden band, we assume a Boltzmann distribution adequately describes the density of electrons in this region of the structure [6] .

$$\Delta N = N_v \left(\frac{m}{2kT} \right)^{1/2} \exp \left(- \frac{m v_x}{kT} \right) \Delta v_x . \quad (1-11)$$

Here we describe the density of valence band electrons with an x-axis directed velocity between v_x and $(v_x + \Delta v_x)$ that are attempting to enter the metallic conduction band.

Clearly, if the density of unoccupied states, Eq.1-10, exceeds the density of excited valence electrons, Eq.1-11, all can enter the conduction band. If, instead, the available electrons with a velocity v_x exceed the number of available unoccupied energy states, many will return to the valence band. For the purpose of this analysis we define a transition energy E_t . The transition energy is that energy bounding these two forementioned energy regions. At energies above E_t the rate at which electrons enter the conduction band is determined by the Maxwellian distribution of valence electrons, Eq.1-11. At energies below E_t the rate at which electrons enter the conduction band is determined by the availability of unoccupied energy states.

Figure 11 through Figure 14 illustrates the calculated value of E_t , described in terms of a barrier energy $W_c = (E_t - E_b)$. Because this transition barrier energy is not unlike the classical Schottky interface energy barrier W_c where $W_c = E_f - E_b$, we have related the two in these illustrative calculations. Classical theory is based upon an assumption that excited valence electrons must reach an energy E_f to enter the conduction band; this is equivalent to the general concept that a hole at E_f moves to E_b . Contrasting with this classical concept the transition barrier W_c represents the energy to which valence electrons must be excited for all to enter the conduction band. Below W_c their entry into the conduction band is governed by the availability of unoccupied energy states.

From these illustrations, Fig.11 through Fig.14, it is clear that the transition energy W_c is significantly lower than the classical barrier W_c , for all values of free electron density. It is through calculations of the

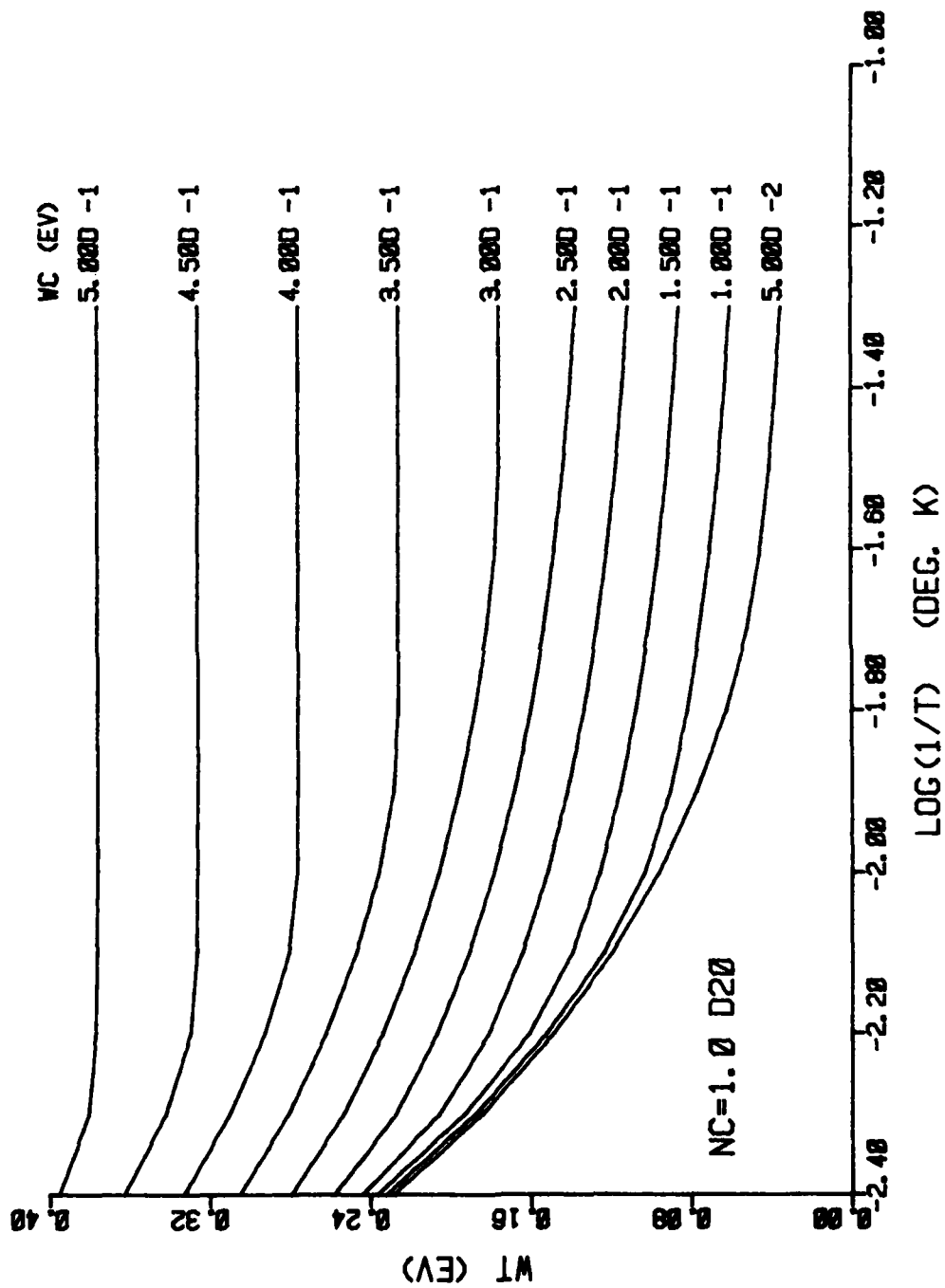


Fig.11 Calculated Transition Barrier W_t in a p-type Schottky Device

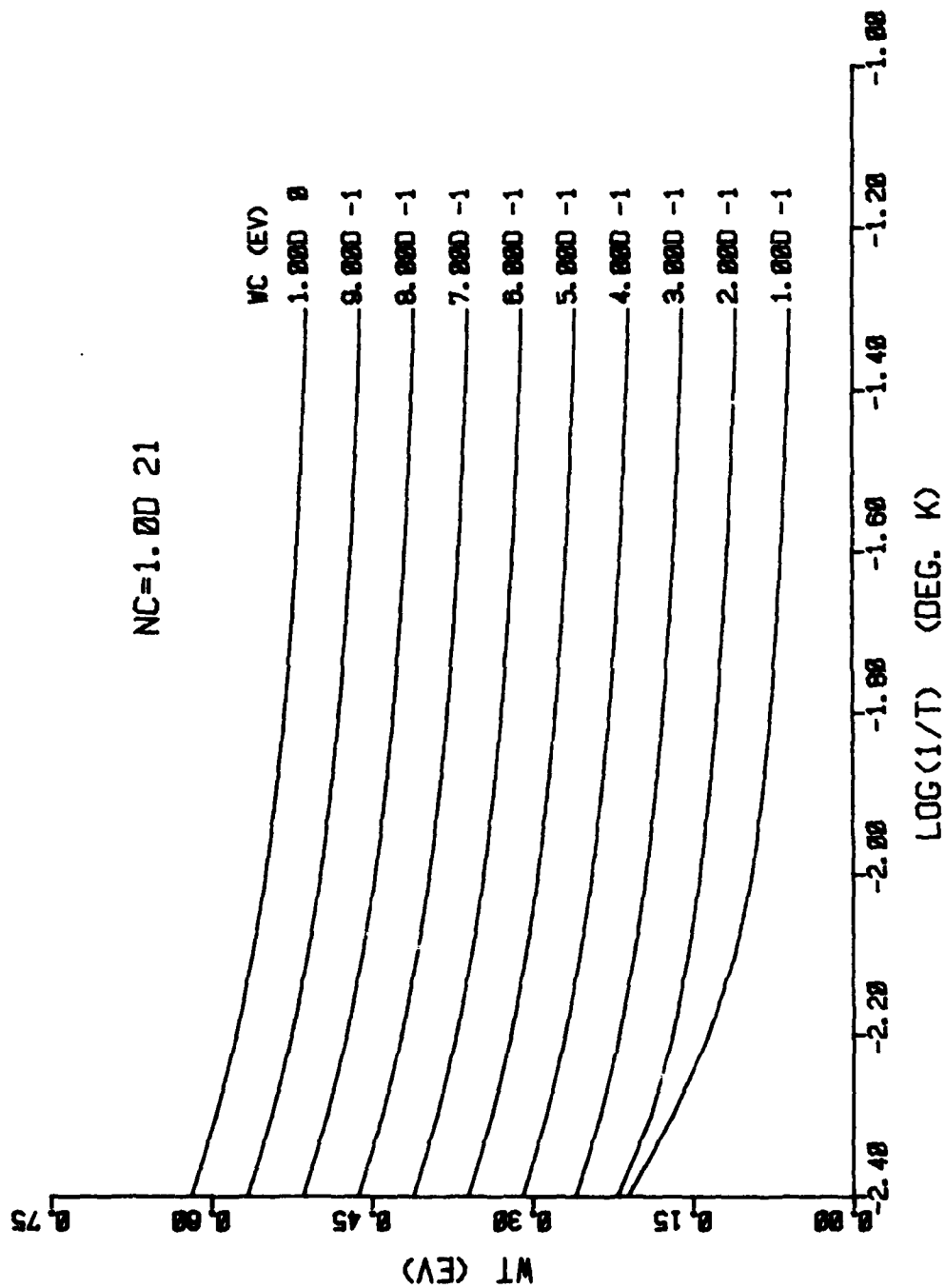


Fig.12 Calculated Transition Barrier W_t in a p-type Schottky Device

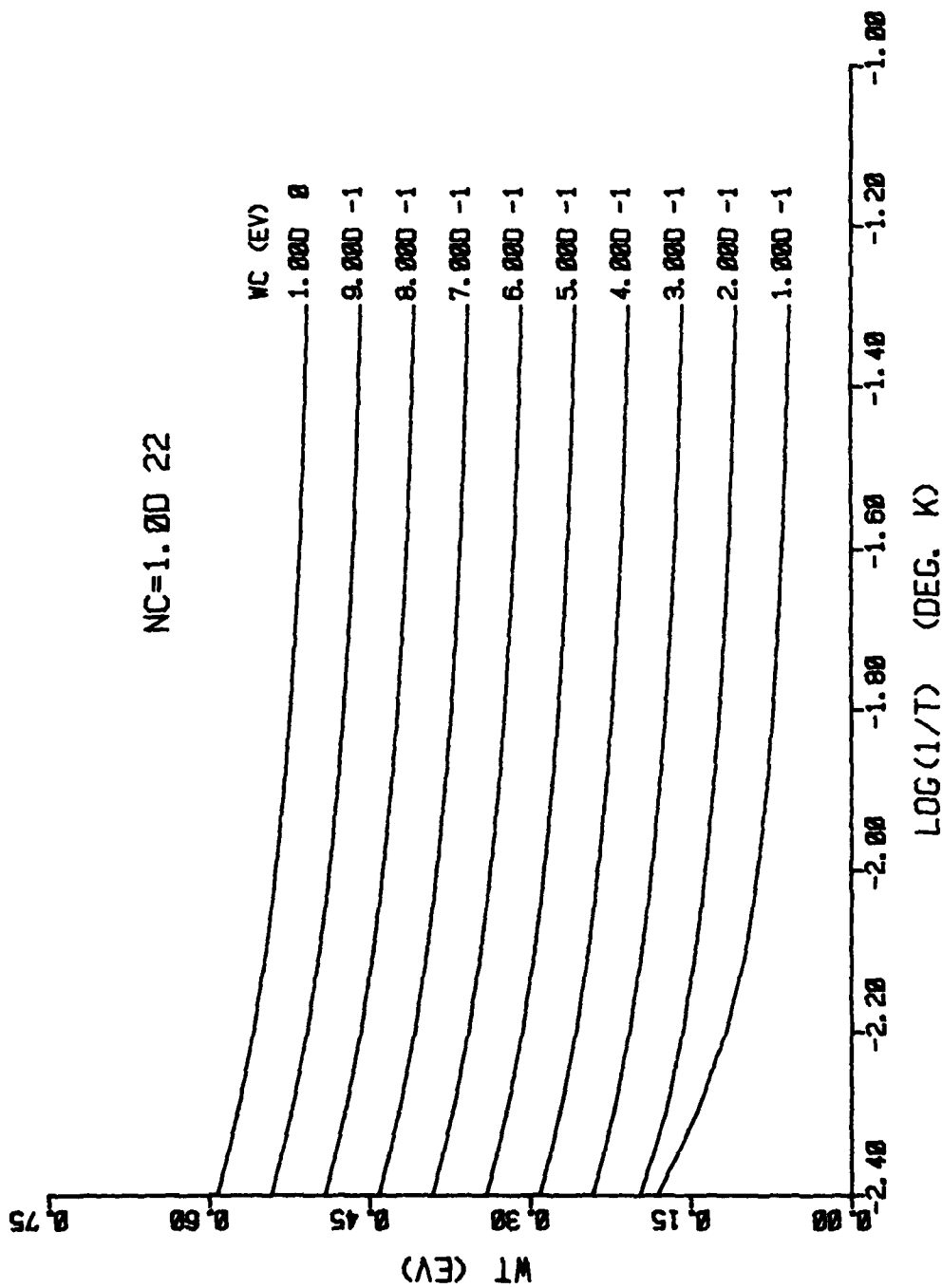


Fig.13 Calculated Transition Barrier W_t in a p-type Schottky Device

barrier electric current above and below the transition energy E_t we shall establish the reverse electric current in a p-type Schottky barrier.

5.0 The Electric Current in a Schottky Barrier---Classical Concept

The classical concept of p-type Schottky diode operation is that the total electric current can be represented by an expression of the form

$$J = J_0 \left[1 - \exp (-q V_a / k T) \right] , \quad (1-12)$$

where V_a is an applied voltage and J_0 is the saturation current.

To date, a rigorous calculation for J_0 has not been found in the technical literature. It is an accepted practice to attribute J_0 to two distinctly different mechanisms: first, hole-electron generation in the p-type semiconductor material and, second, hole transitions from the metal to the semiconductor material. The first mechanism can be acknowledged as well founded but, instead, there remains no real quantitative explanation for the saturation current at low temperatures; at temperatures that render hole-electron generation insignificant.

In order to adequately evaluate our concept of p-type device operation it is necessary to recast this classical theory into a form suitable for comparison. For this reason we abandon the notion of hole generation in the metal and consider this traditional theory in terms of valence electron excitation to the Fermi-level. Clearly, this is consistent with the concept of hole transitions from the Fermi-level to the valence band.

As in Section 4.0 of this chapter, we assume a Maxwellian velocity distribution for valence electrons given by

$$\Delta N = N_v \left(\frac{m}{2\pi k T} \right)^{1/2} \exp \left(- \frac{1}{2} m v_x^2 / k T \right) \Delta v_x \quad (1-13)$$

Further, we assume an electric current produced by this velocity distribution given by

$$J_o = q \int_{v_f}^{\infty} v_x dn = q N_v \left(\frac{k T}{2 m^*} \right)^{1/2} \exp \left(-E_f / k T \right) , \quad (1-14)$$

where

$$v_f = (2 E_f / k T) . \quad (1-15)$$

Equation (1-14) represents an expression for the saturation current J_o that retains the traditional concept of hole transitions from the Fermi-level to the conduction band. Nonetheless, this expression has been developed in a manner that we believe is quantitatively reasonable, and can be used for comparison with new concepts of device operation arising from the present research.

In the foregoing equations N_v represents the density of valence electrons that are at an energy in excess of the valence band edge at the metal-semiconductor interface, E_b . This is easily calculated if we first determine the location of E_v , relative to the lower edge of the valence band.

The density of occupied energy states in a semiconductor is given by

$$N = 8\pi \sqrt{2} \left(\frac{\sqrt{m}}{h} \right)^3 \left(\frac{m^*}{m} \right)^{3/2} \int_0^{E_v} \frac{\sqrt{E} dE}{1 - \exp (E - E_f) / k T} . \quad (1-16)$$

If we assume a temperature of zero degrees K, the Fermi-level is essentially at E_v , and we have

$$N_t = 8\pi \sqrt{2} \left(\frac{\sqrt{m}}{h} \right)^3 \left(\frac{m^*}{m} \right)^{3/2} \frac{3}{2} E_{f0}^{-3/2} \quad (1-17)$$

where N_t is the total number of valence electrons, and E_{f0} is the Fermi-level (at 0° K) as measured with respect to the lower boundary of the valence band. Because at the interface E_{f0} and E_b coincide, we can now state that the density of unoccupied states in the valence band is

$$N_v = \frac{3}{2} E_{f0}^{-3/2} \int_0^{E_{f0}} \frac{\sqrt{E} dE}{1 + \exp(E'_f + E) / kT} \quad (1-18)$$

where E'_f is the interface Fermi-level when measured with respect to the lower edge of the semiconductor conduction band,

$$E'_f = E_{f0} + (E_f - E_b) \quad (1-19)$$

Because valence electrons not found in the valence band must be at an energy in excess of E_b , we know the number of electrons involved in the Maxwellian distribution and, hence, N_v for Eqs.(1-12) and(1-13).

6.0 Reverse Current From Transitions Above E_t

As outlined in Section 4.0, electron excitation from the valence band E_b , Fig.1, to an energy above E_t (the transition energy) will assure a transition into the metal. Hence, like the traditional theory, we can immediately establish this component of the diode saturation current through a minor

modification of Eq.1-14.

$$J_1 = q \int_{v_t}^{\infty} v_x dn = q N_v \left(\frac{k T}{2 \pi m} \right)^{\frac{1}{2}} \exp \left(-E_t / k T \right) \quad (1-20)$$

where

$$v_t = (2 E_t / m)^{\frac{1}{2}} \quad (1-21)$$

This expression has been used in all of the following calculations as one component of the total saturation current J_o , and N_v is determined using Eq.1-18.

7.0 Reverse Current From Transitions Below E_t

Below the transition energy E_t the density of unoccupied energy states becomes less than the number of electrons available to occupy these states. If we recast the density of unoccupied states into an expression for electron velocity, Eq.1-10, we obtain

$$\Delta N = N_c \frac{3}{2} (E_{f0} / m)^{-3/2} v^2 \left[1 + \exp (E_f - \frac{1}{2} m v^2) \right]^{-1} dv \quad (1-22)$$

Thus, the electric current produced by transitions to these energy states is given by

$$J_2 = q N_c \frac{3}{2} (E_{f0} / m)^{-3/2} \int_0^{v_t} \frac{v^3 dv}{1 + \exp (E_f - \frac{1}{2} m v^2)} \quad (1-23)$$

where

$$v_t = (2 E_t / m)^{1/2} \quad (1-24)$$

Rewriting Eq.1-19 into energy we obtain

$$J_2 = 3qN_c E_{f0}^{-3/2} m^{-1/2} \int_0^{E_t} \frac{E dE}{1 + \exp (E_f - E) / k T} \quad (1-25)$$

Equation (1-21) is the expression we use for calculating the electric current produced by electron transitions below the transition energy E_t .

8.0 Computations of Reverse Electric Current

Few, if any, of the foregoing equations can be evaluated on an analytical basis; integration of the Fermi-Dirac distribution equation must be done numerically, on a computer. For this reason, our initial evaluation of this new concept of Schottky barrier operation has been accomplished through a sequence of electric current calculations. Equation (1-20) and Eq.(1-25) have been used for calculating the current predicted by these new theoretical concepts, and such calculations are compared with those using Eq.1-14 as representative of the classical theory for Schottky diode operation.

Figure 15 through 18 illustrate the total reverse current predicted by Eq.(1-20) and Eq.(1-21) for J_1 and J_2 respectively, throughout a wide assumed range for the free electron density in the metal conduction band. A comparison is first undertaken between these calculations Fig.15 through Fig.18, and similar calculations based upon classical theory, Fig.19 and Fig.20. Because W_c is given in these calculations ($W_c = E_f - E_b$), classical

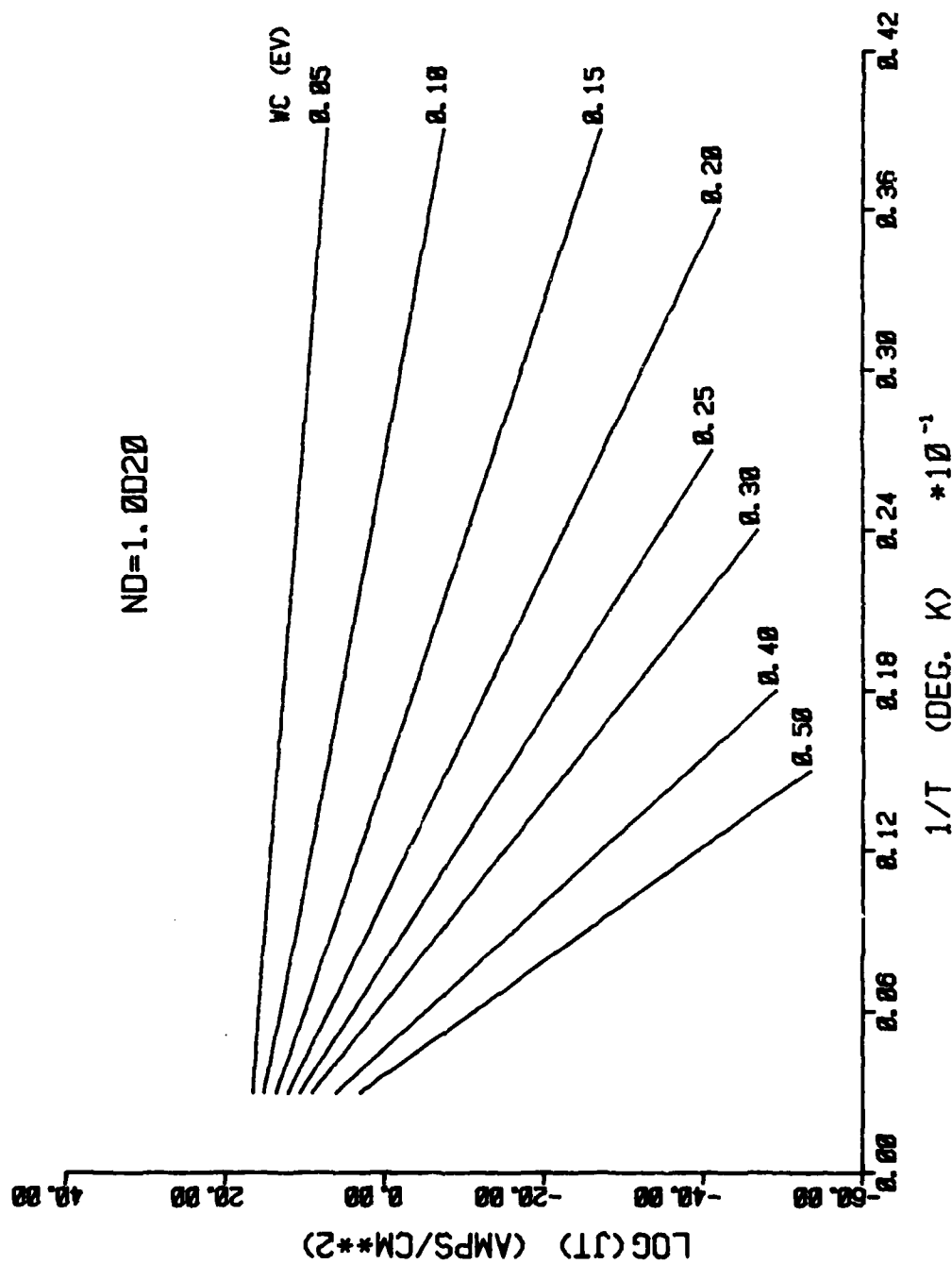


Fig.14 Calculated Total Saturation Current for a Range of Assumed Barrier Height, W_c

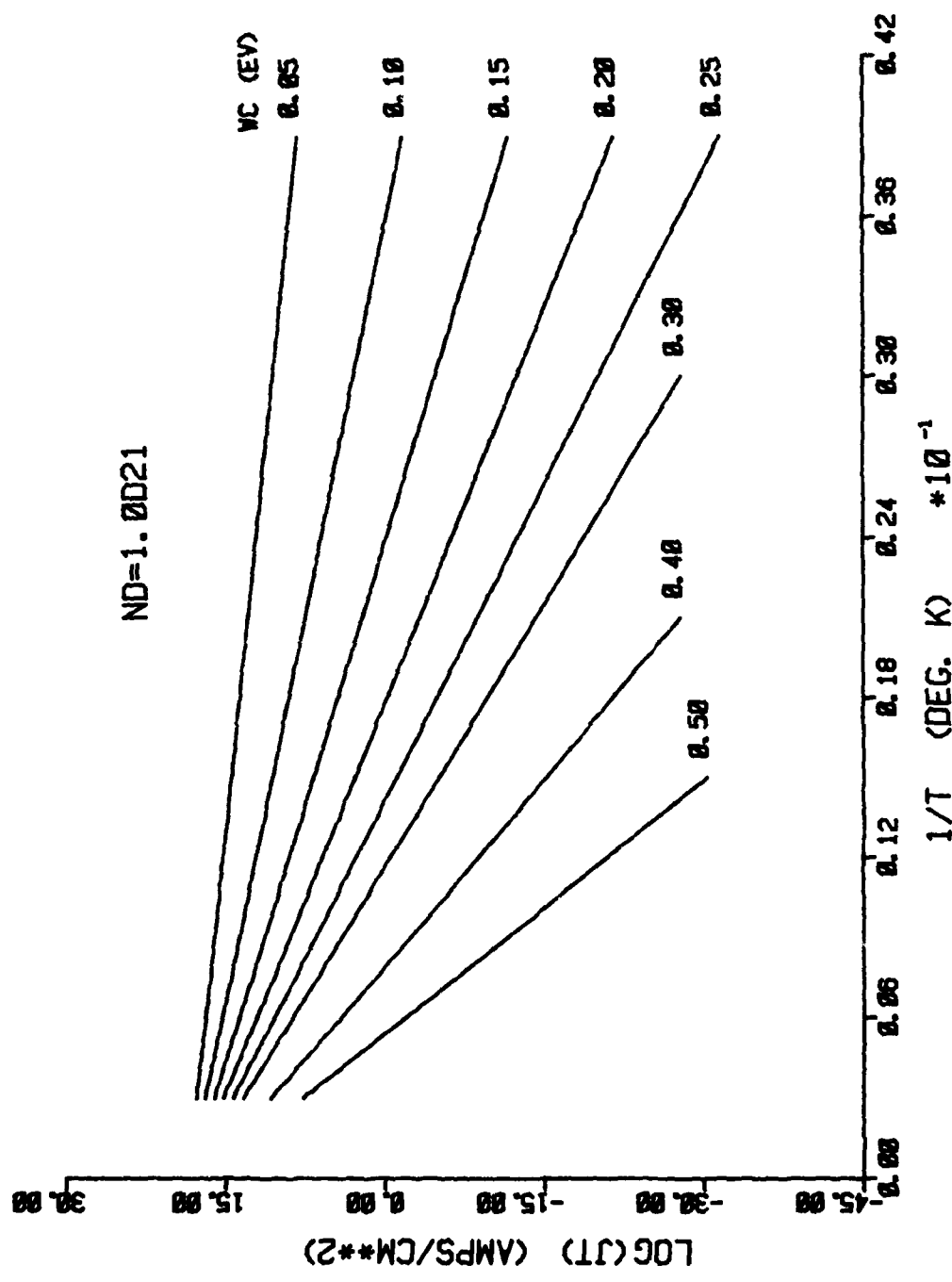


Fig.15 Calculated Total Saturation Current for a Range of Assumed Barrier Height, W_c

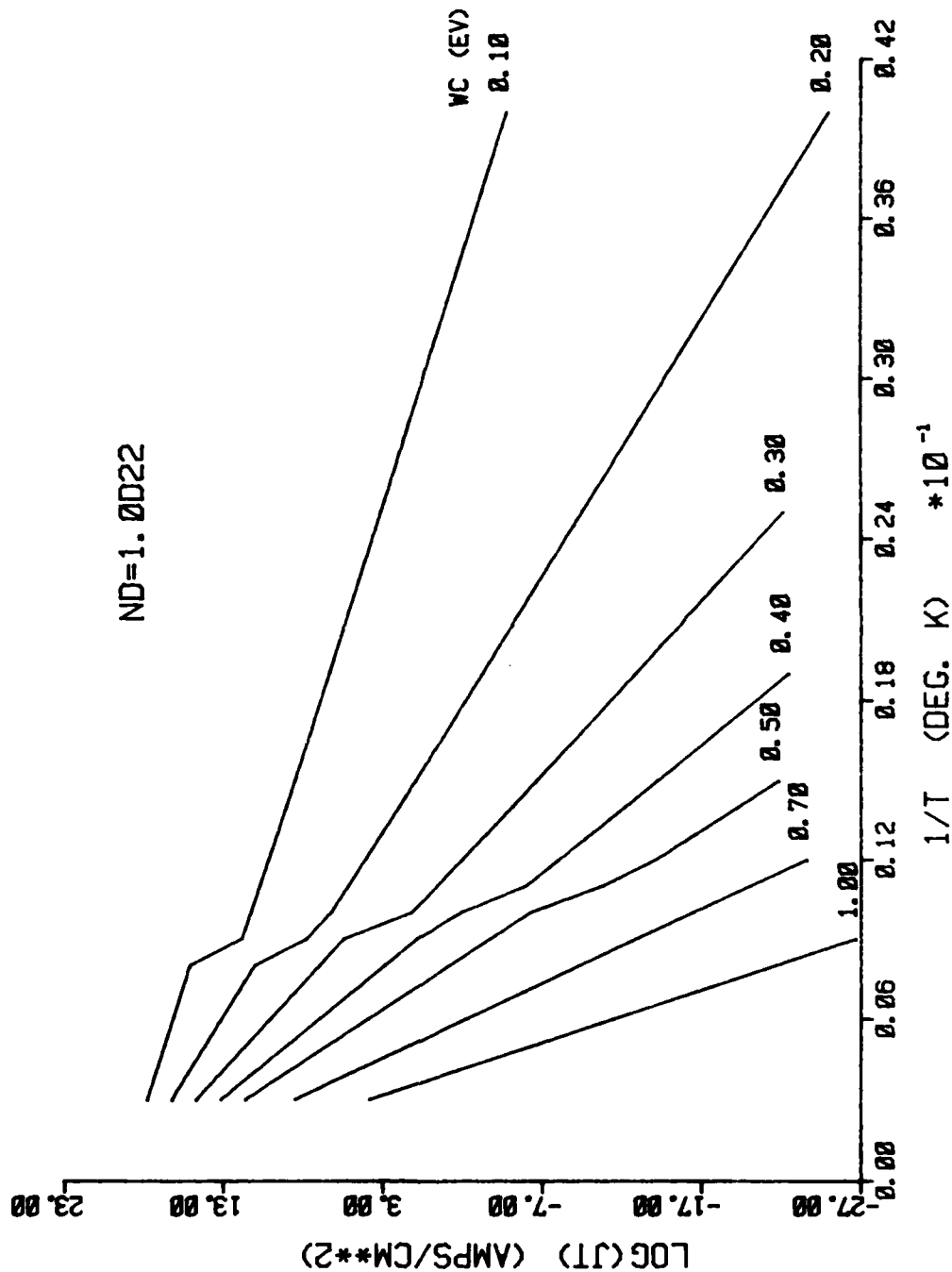


Fig.16 Calculated Total Saturation Current for a Range of Assumed Barrier Height, W_c

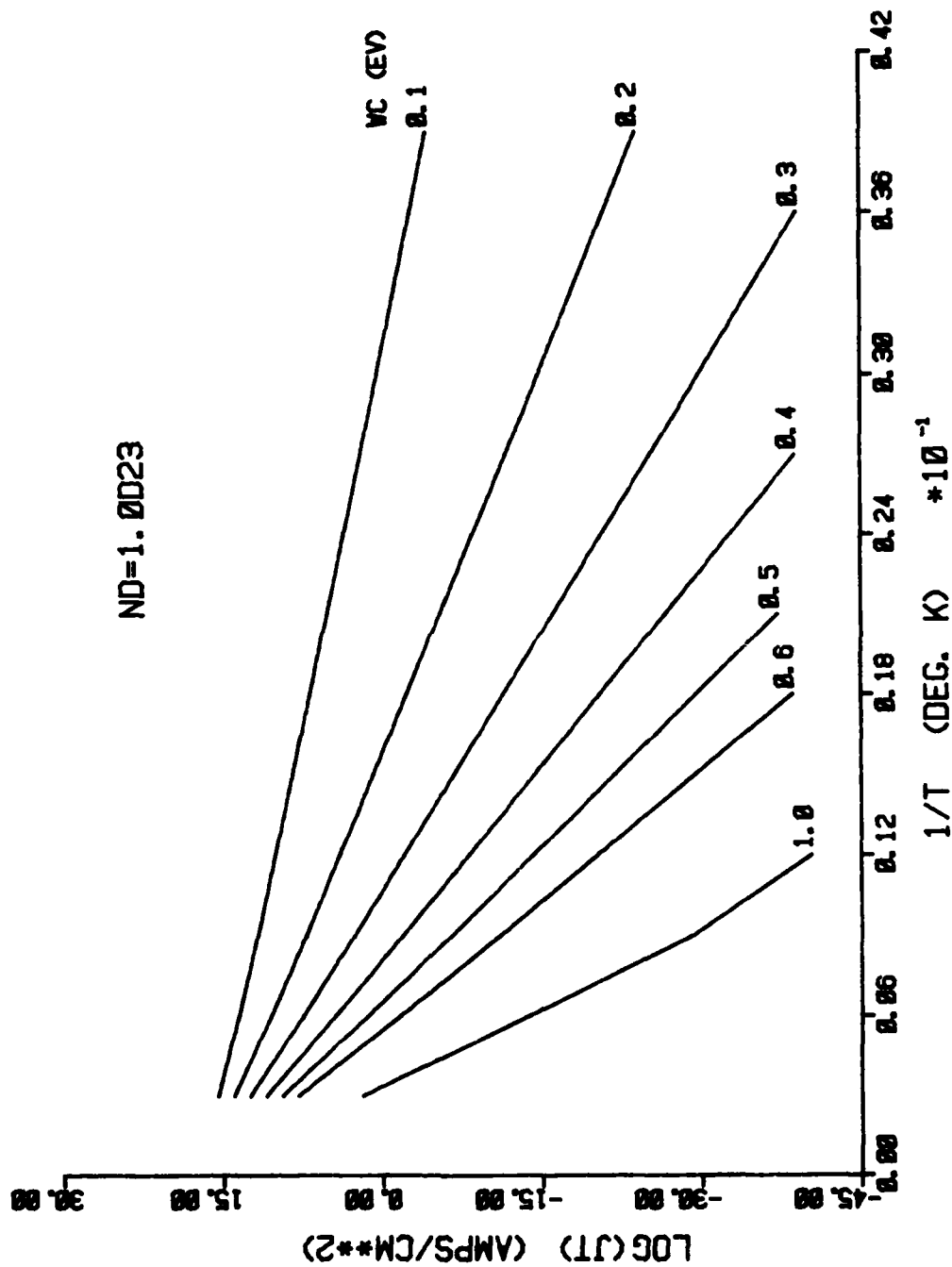


Fig. 17 Calculated Total Saturation Current for a Range of Assumed Barrier Height, W_c

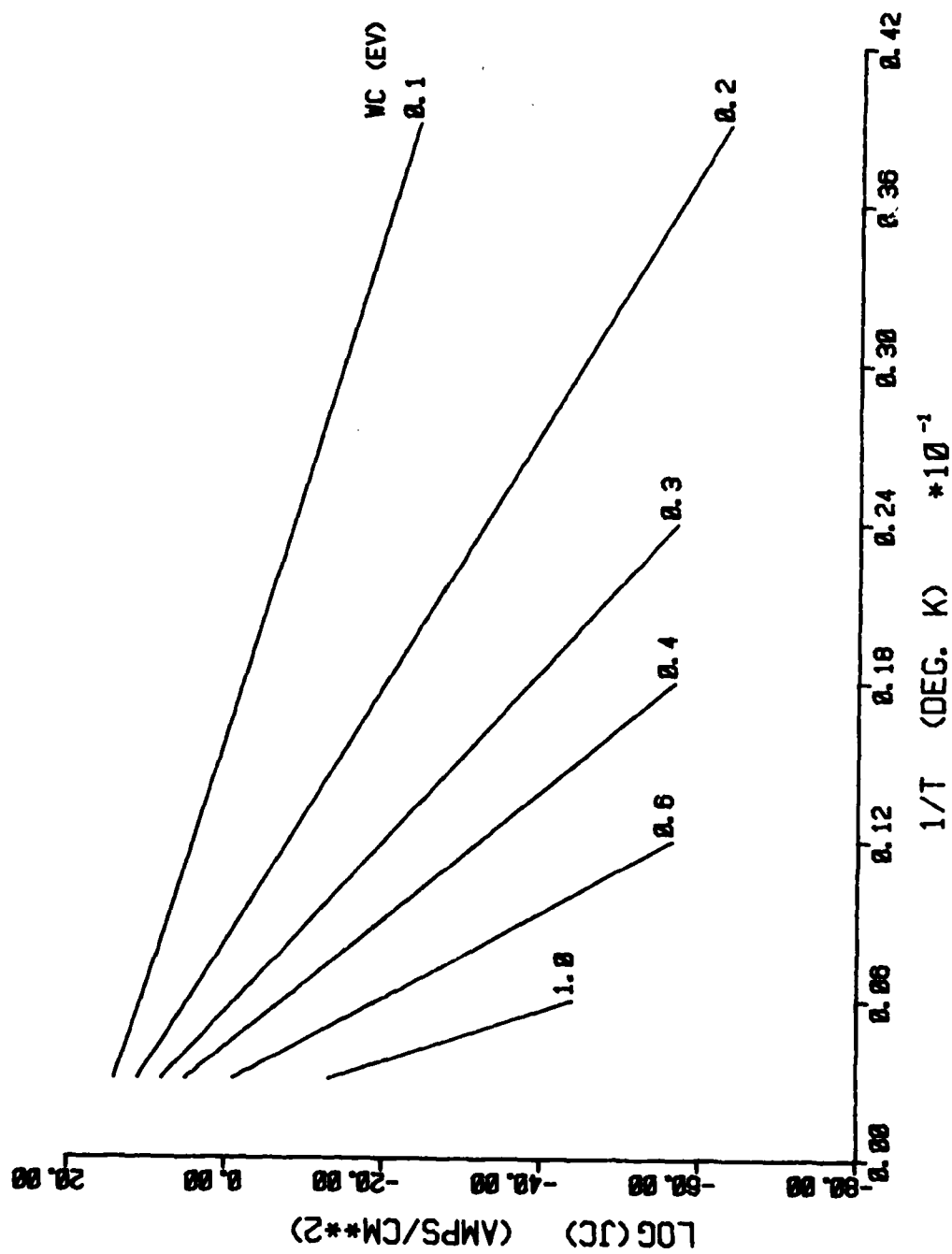


Fig.18 Calculated Diode Current Using Classical Theory

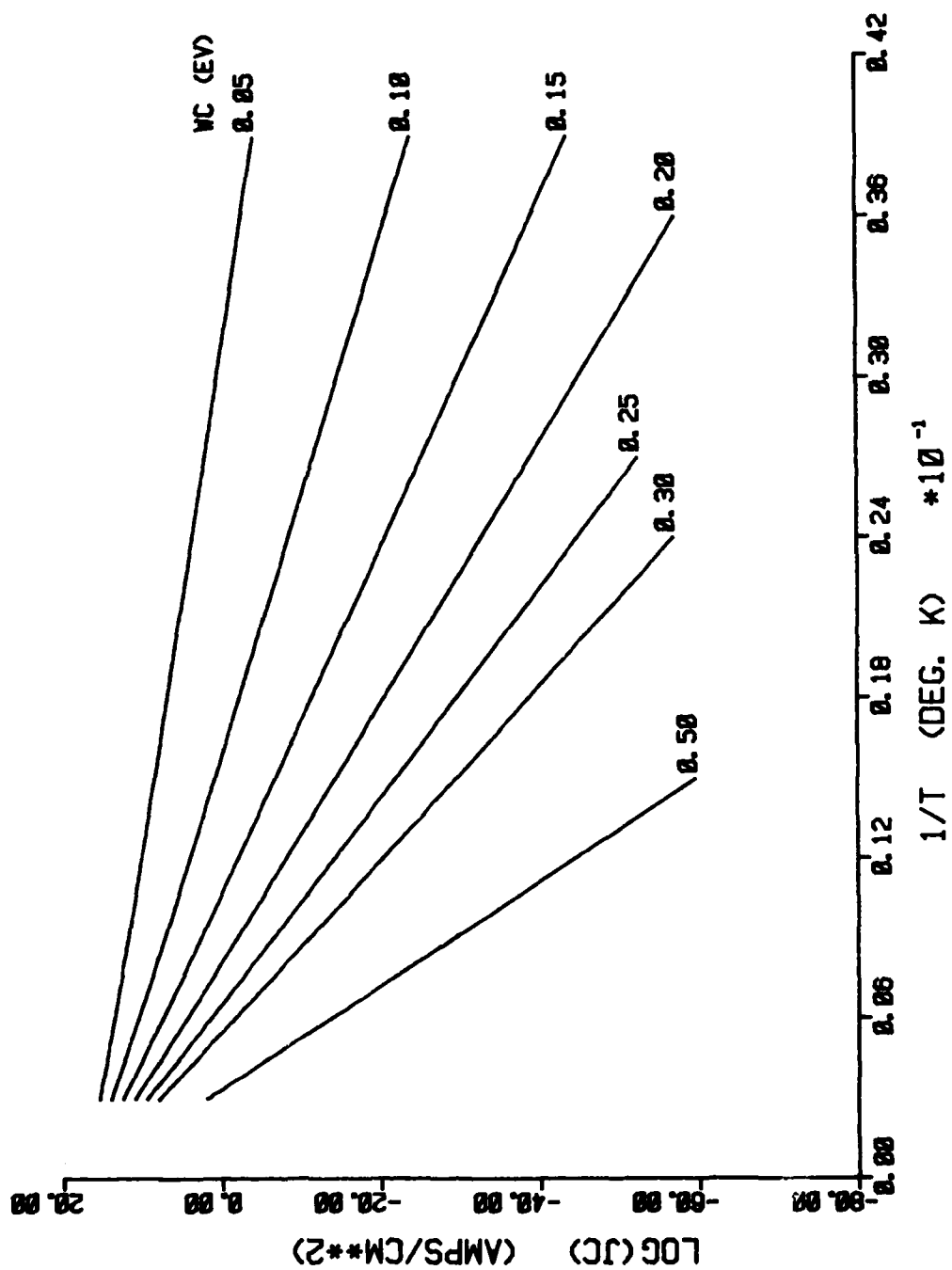


Fig.19 Calculated Diode Current Using Classical Theory

theory is nearly independent of the free electron density in the metal and, hence, only a single illustration is needed for J_c . For convenience, J_c is presented in two illustrations, Fig.19 and Fig.20, which have different assumed ranges for W_c .

We encounter two different situations in these calculations with relation to N_c , the conduction band electron density: first, when N_c is small ($N_c \approx 10^{20}$) and, second, when N_c is large ($N_c \approx 10^{23}$). When N_c is small the metallic conduction band closely resembles that of a highly degenerate n-type semiconductor; the Fermi-level is only a small distance above the conduction band edge, E_c . As a consequence, many of the assumed values for barrier energy W_c places the semiconductor valence band edge, E_b , below the conduction band edge, E_c . In the second case ($N_c \approx 10^{23}$) we have a metallic conductor in which the Fermi-level is well above the conduction band edge and, therefore, any reasonable assumption for W_c ($W_c \leq \approx 1.0$ ev) places the semiconductor valence band edge at the interface, E_b , well within the metal conduction band ($E_c \leq E_b \leq E_f$).

Calculations show that by assuming $N_c = 10^{20}$, this new theory of operation yields a reverse current, J_t , that is always substantially larger than that given by classical theory, J_c . For purposes of comparison, some illustrative calculations yield at $T = 60^\circ K$:

W_c (ev)	J_t (amps/cm ²)	J_c (amps/cm ²)
0.5	10^{-53}	10^{-60}
0.3	10^{-23}	10^{-29}
0.25	10^{-15}	10^{-22}
0.2	10^{-8}	10^{-14}

Because in the foregoing calculations E_b lies below the conduction band edge no contribution to J_t arises from direct electron transitions from the valence band to the conduction band; all transitions are due to thermally excited valence electrons with an energy in excess of E_b . For $N_c = 10^{20}(\text{cm}^{-3})$,

only at an assumed barrier of .05 ev ($W_c = 0.05$) does this direct transition mechanism produce an electric current, J_2 , that contributes significantly to J_t , Fig.25. For this low barrier situation ($W_c = 0.05$ ev) we calculate:

<u>T(°K)</u>	<u>J_1</u>	<u>J_2</u>	<u>J_t</u>	<u>J_c</u>
27	$10^{5.5}$	$10^{7.9}$	$10^{7.9}$	$10^{-4.2}$
30	$10^{6.3}$	$10^{8.7}$	$10^{8.7}$	$10^{-2.7}$
33	$10^{7.1}$	$10^{9.4}$	$10^{9.4}$	$10^{-1.1}$
41	$10^{7.9}$	$10^{10.2}$	$10^{10.2}$	$10^{4.0}$
47	$10^{8.7}$	10^{11}	10^{11}	10^{19}
55	$10^{9.6}$	$10^{11.8}$	$10^{11.8}$	10^{35}
66	$10^{10.4}$	$10^{12.5}$	$10^{12.6}$	10^{51}

Contrasting with the foregoing small free electron situation, by assuming $N_c = 10^{23}$ (cm^{-3}) the Fermi-level is moved well away from the conduction band edge. As with $N_c = 10^{20}$ we again obtain a small electric current component due to direct transitions, but for an entirely different reason. Setting $N_c = 10^{23}$ places the interface valence band energy, E_b , well within the metallic conduction band edge which, under the proper circumstances, could produce a large direct transition current. When $N_c = 10^{23}$ we find that unoccupied conduction band energy states are clustered within a small energy range from E_f . As a consequence, when E_c is sufficiently large we obtain a negligible amount of current due to direct electron transition from the valence band to the conduction band.

For the purposes of illustration, the following represent the calculated electric current at $T = 83^\circ \text{K}$:

<u>W_c (ev)</u>	<u>J_t</u>	<u>J_1</u>	<u>J_c</u>
0.6	10^{-20}	10^{-20}	10^{-56}
0.5	10^{-14}	10^{-14}	10^{-32}
0.3	10^{-2}	10^{-2}	10^{-20}
0.2	10^4	10^4	10^{-8}
0.1	10^{10}	10^{10}	10^{-4}

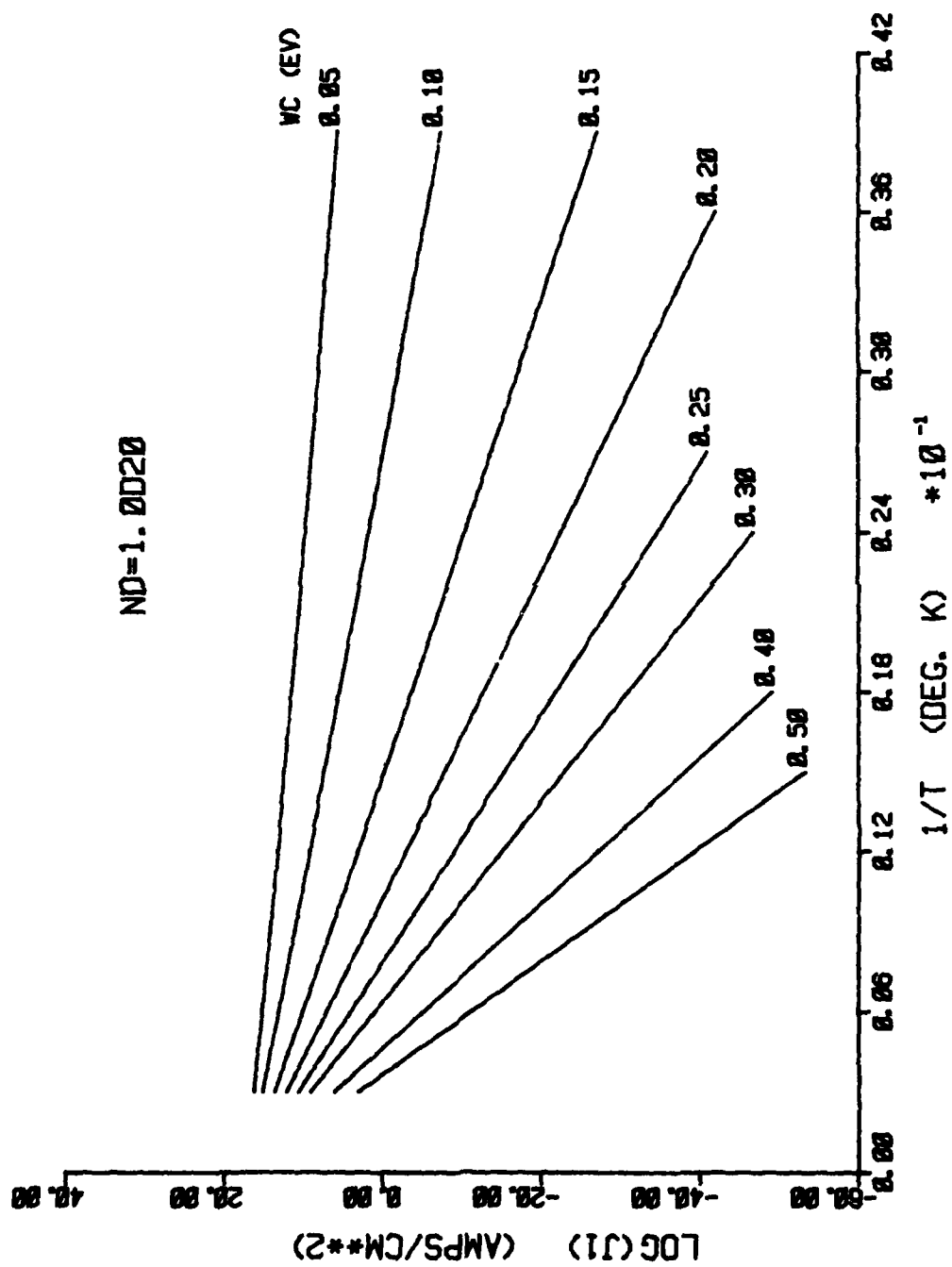


Fig.20 Saturation Current Component Due to Transition of Electrons with an Energy Greater Than E_t

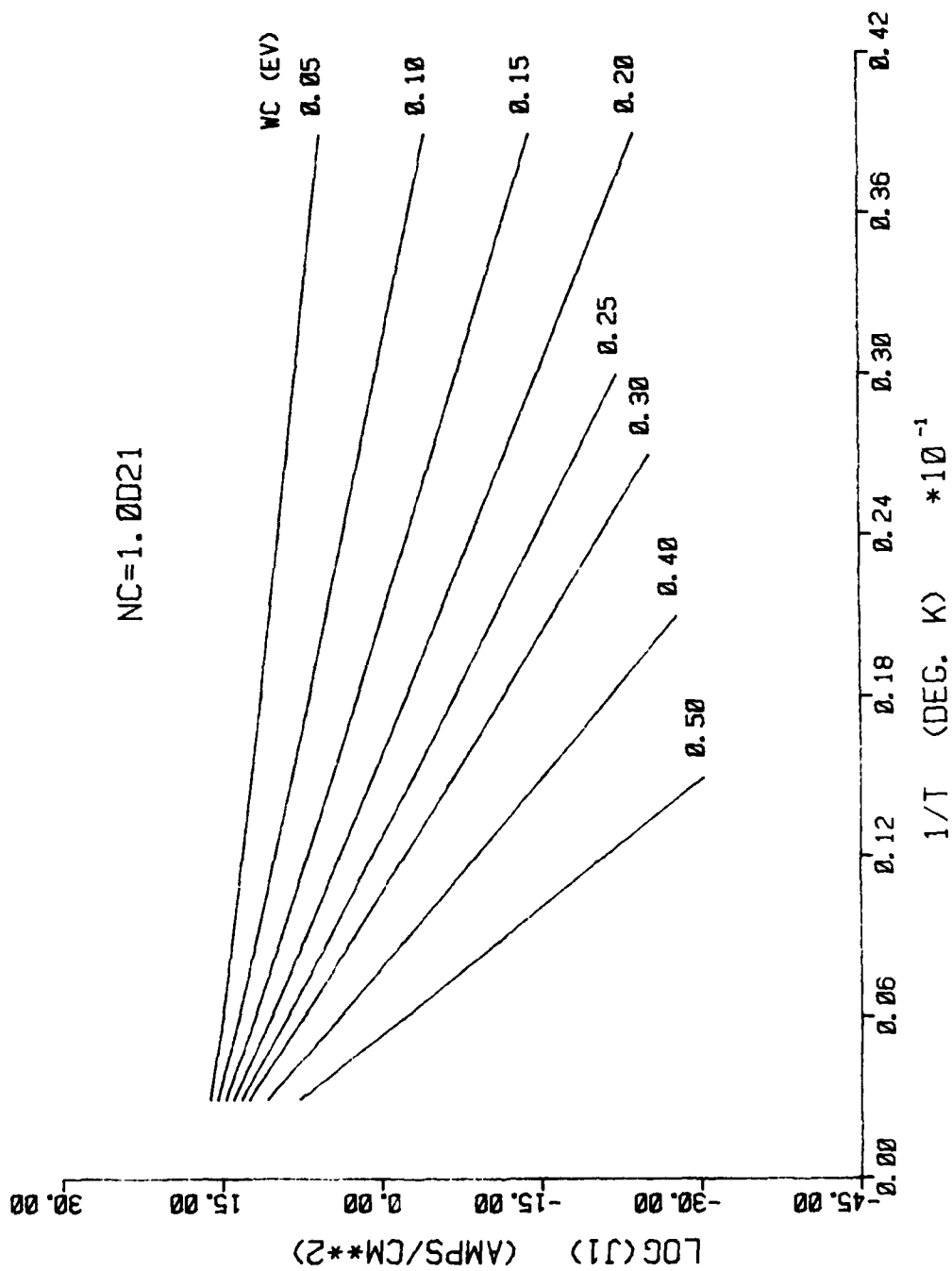


Fig. 21 Saturation Current Component Due to Transition of Electrons with an Energy Greater Than E_t

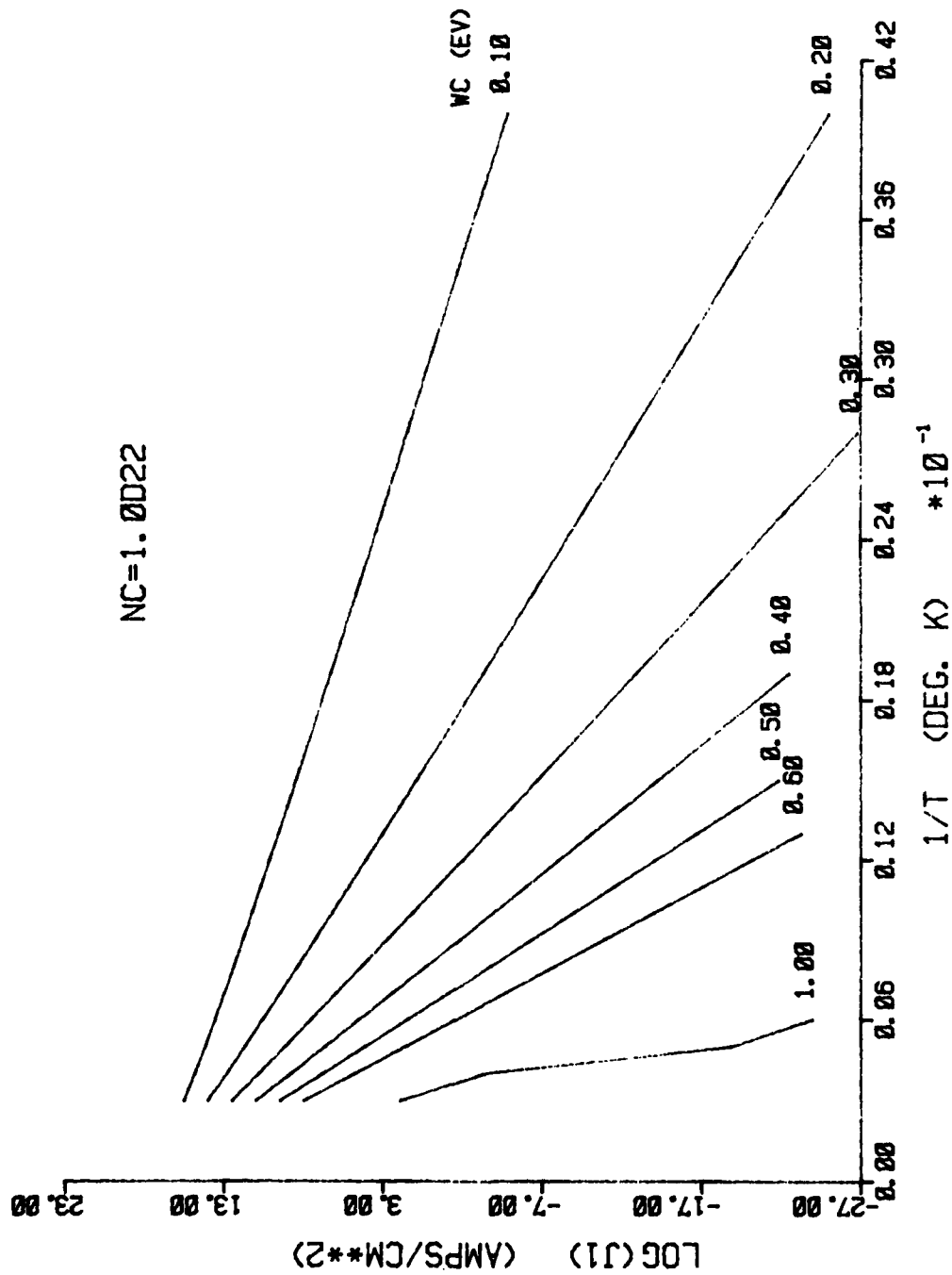


Fig. 22 Saturation Current Component Due to Electrons with an Energy Greater Than E_t

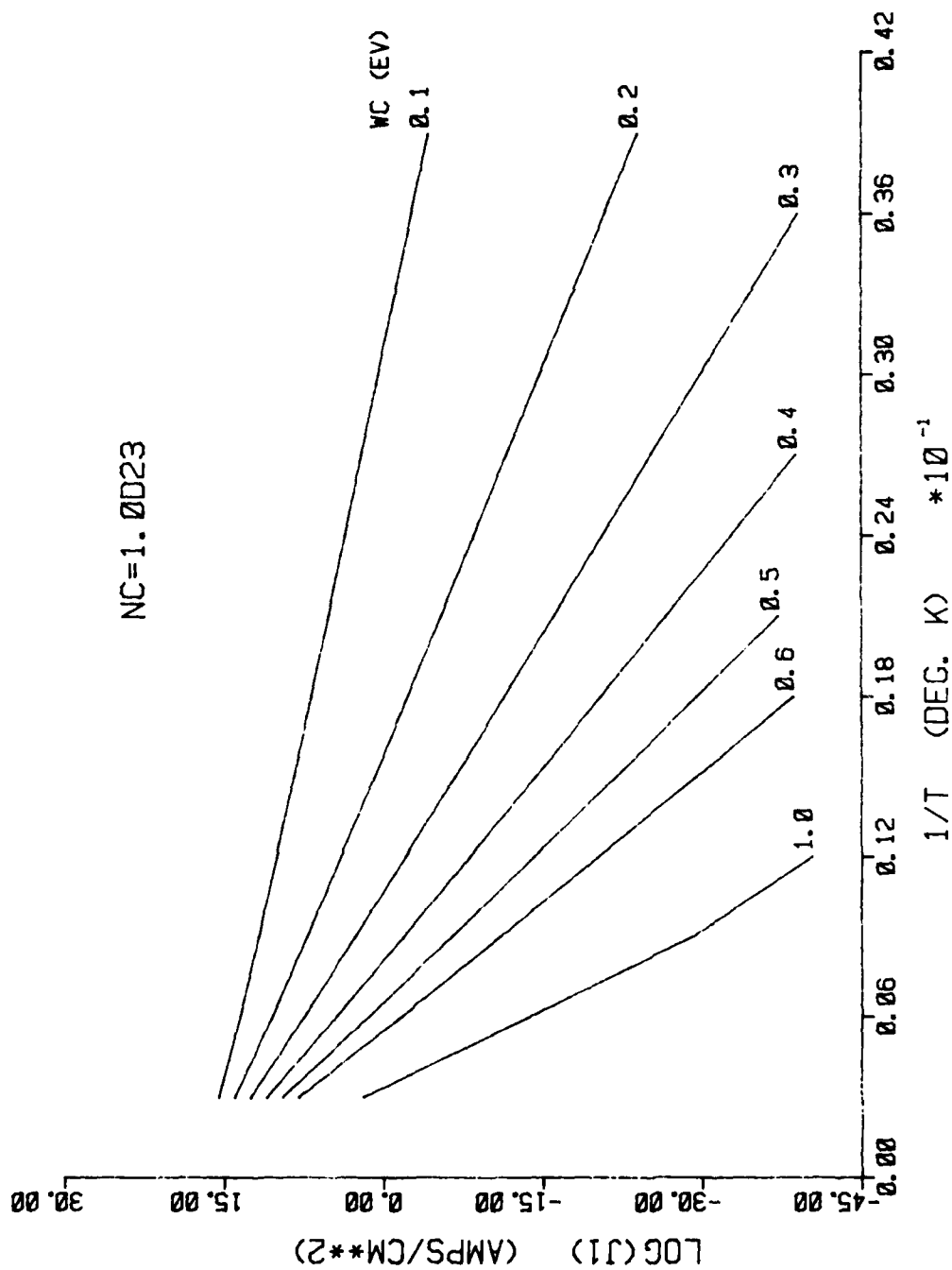


Fig. 23 Saturation Current Component Due to Electrons with an Energy Greater Than E_t

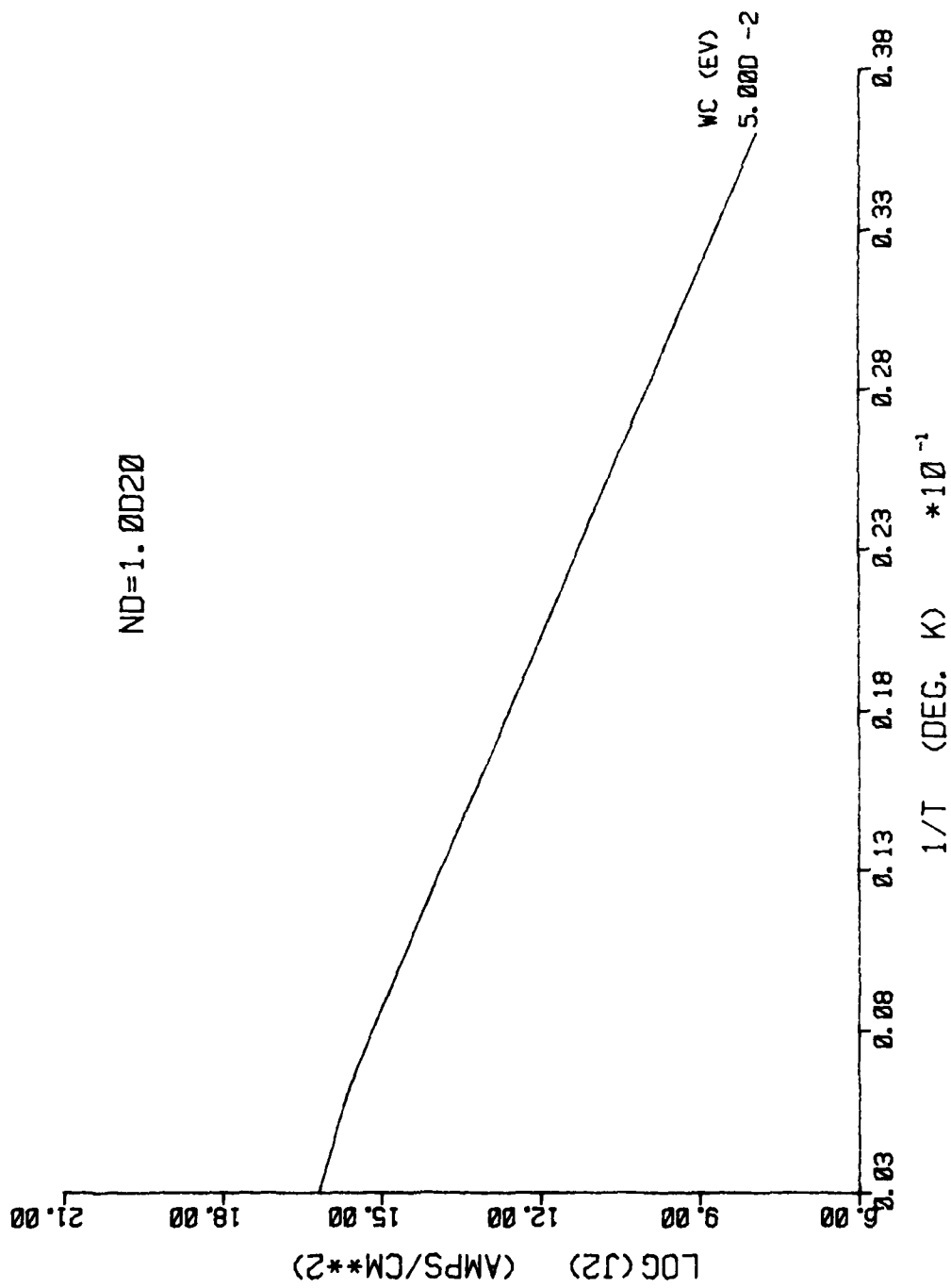


Fig. 24 Saturation Current Component Due to Transitions by Electrons with an Energy Less Than E_t

where current is in amps/cm². In all of these calculations the direct transition current remained relatively unchanged at 10⁻⁴⁷ amps/cm²; this situation probably arises from underflow protection within the computer program. This sequence of calculations indicate that very few unoccupied states reside in lower regions of the conduction band when $N_c = 10^{23}$. Nonetheless, a sufficient number exist below E_f so that J_t is significantly larger than J_c .

An intermediate range is found between $N_c = 10^{20}$ and $N_c = 10^{23}$ where both J_1 and J_2 can contribute in a significant fashion to the total electric current. In this intermediate region, where $10^{20} < N_c < 10^{23}$, the unoccupied energy states can reside at energy levels far below the Fermi-level, E_f . As a consequence of this situation the transition energy E_t can reside well below E_f and, therefore, $W_t < W_c$, which assures $J_c < J_1$. Additionally, a large number of unoccupied energy states can reside below the transition barrier W_t , and this situation implies a direct transition current J_2 that can be significant.

We first consider the electric current calculated for an assumed free electron density N_c of 10²¹ (cm⁻³). At 66° K our calculations yield the following results:

W_c (ev)	J_t	J_1	J_2	J_c
0.30	10 ⁻⁵	10 ⁻⁶	10 ⁻⁵	10 ⁻²⁹
0.20	10 ^{2.8}	10 ^{0.8}	10 ^{2.8}	10 ⁻¹⁴
0.10	10 ¹⁰	10 ^{8.4}	10 ¹⁰	10 ^{0.8}

where all current is in amps/cm³. In this situation two different (although related) mechanisms contribute to the total electric current J_t . Transitions of thermally excited electrons to unoccupied energy states produce an electric current component J_1 that is significantly greater than predicted from classical concepts, J_c . This situation implies that the transition to unoccupied energy states below E_f ($E_t \leq E \leq E_f$) occurs at a greater rate than transition to unoccupied states above E_f ($E_f \leq E \leq \infty$). These calculations also show that transitions with no apparent thermal excitation

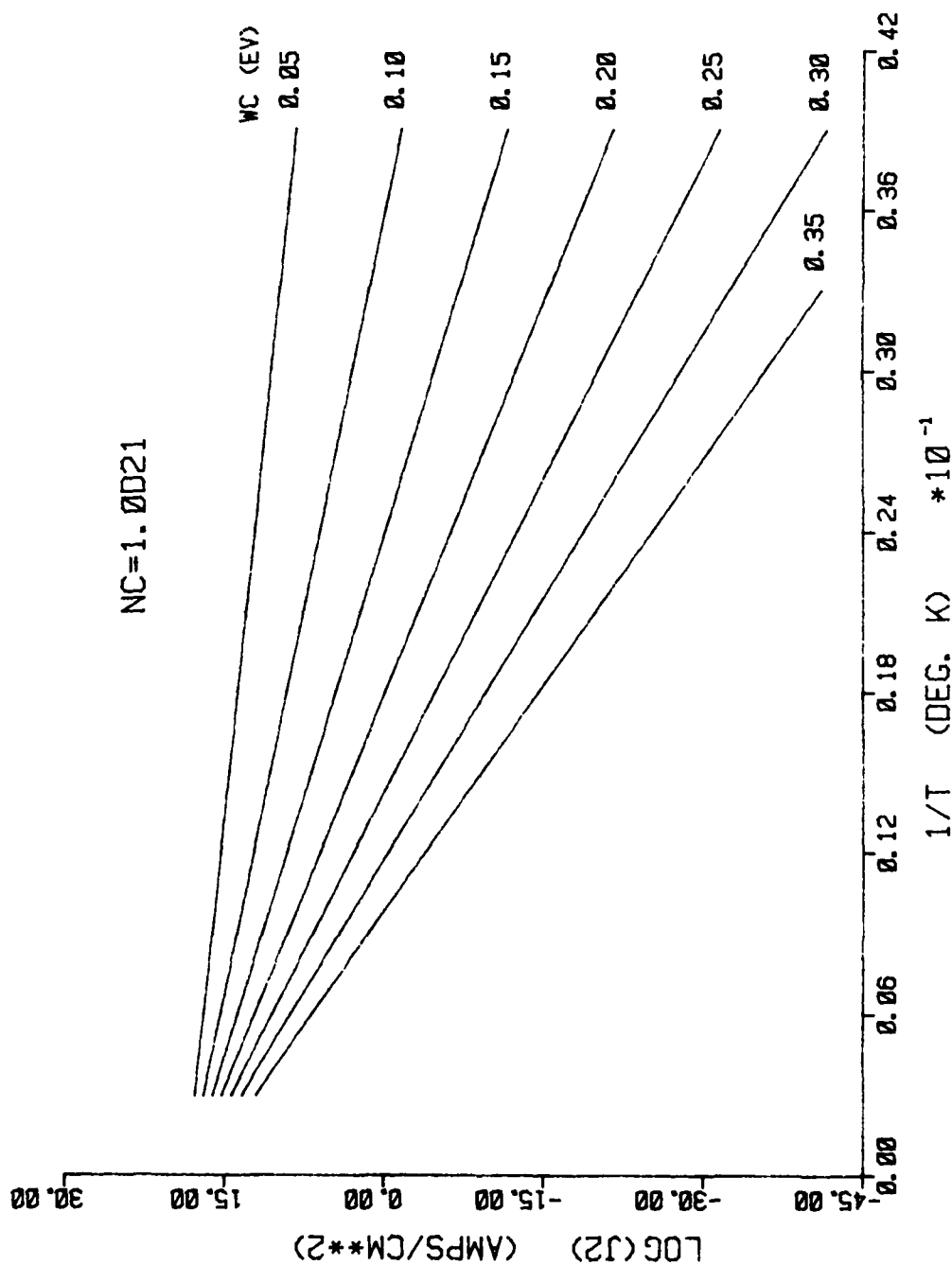


Fig.25 Saturation Current Component Due to Transitions by
Electrons with an Energy Less Than E_t

($E_c \leq E \leq E_t$) take place at a rate that is significantly greater than the transition of thermally excited valence electrons. Hence, in this computational illustration both J_1 and J_2 are significant in magnitude, and in combination they produce a greater electric current than predicted using classical concepts of diode operation.

By assuming $N_c = 10^{22} \text{ (cm}^{-3}\text{)}$ we obtain a Fermi-level that is well above the conduction band edge, yet the distribution of unoccupied states extends for a significant energy range below this Fermi-level. As a consequence, direct transition current J_2 can be very large, Fig.26, in conjunction with a large current J_1 due to transitions above the transition energy E_t , Fig.23. In combination, the total junction current, Fig.17, is much larger than expected from conventional concepts of device operation, Fig.19 and Fig.20.

It should be mentioned that the apparent change of slope in Fig.17 appears to be a real mechanism, and not a problem of the computer program. At high temperature the total current is dominated by direct valence electron transitions to the conduction band and, thereby, determining the total current J_t . A decrease of temperature produces a rapid fall off of this direct transition current, Fig.27, and J_t is determined by transitions above the transition energy E_t . Although it is not shown in these calculations, at a lower temperature many of these curves in Fig.17 exhibit another change of slope; this change is attributed to a rapid decrease of N_v ; the valence electrons residing above the valence band edge, E_b , at the metal-semiconductor interface.

9.0 Reverse Current in a p-type Schottky Barrier at 77°K

In reverse bias situations it is presumed that holes are generated at the metal-semiconductor interface through the foregoing mechanisms. After generation these holes move to charge neutral regions of the p-type

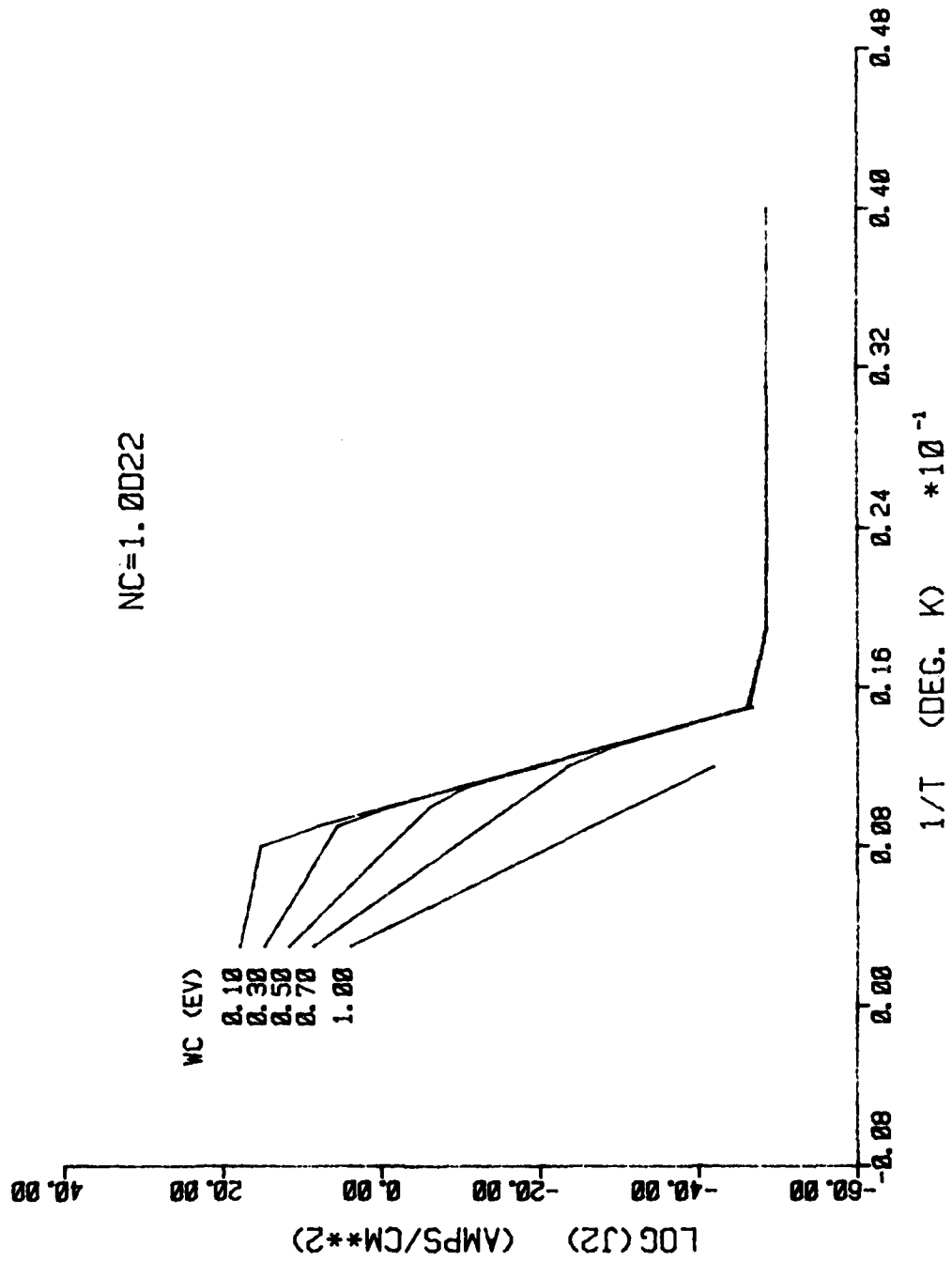


Fig. 26 Saturation Current Component Due to Transitions by
Electrons with an Energy Less Than E_t

material, under the influence of a space-charge electric field; thereby a reverse electric current is produced in this semiconductor device. Experiment shows that the magnitude of this reverse current increases with applied reverse voltage, and this mechanism has not yet been included in the present theory.

From conventional concepts of device operation it can be shown [6] that a lowering of the potential barrier results from the attractive forces between an interface generated hole, and an image charge at the metal. This mechanism is frequently called the Schottky effect, and through this mechanism E_b , Fig.1, will be increased by an amount

$$\frac{1}{2} \sqrt{\frac{q f_o}{\pi \epsilon_o}} \quad , \quad (1-26)$$

where f_o represents the space-charge layer electric field at the metal-semiconductor interface. Using the depletion approximation for determining this electric field, Eq.1-26 has been added to assumed values of E_b yielding a conventional interface energy barrier of

$$W_c = E_f - E_b - \frac{1}{2} \sqrt{q f_o / \pi \epsilon_o} \quad (1-27)$$

We next apply our new theoretical concepts to a reverse biased Pt-Si diode operating at 77° K. Additionally, we compare the results of such calculations with similar calculations using conventional theoretical concepts. It is emphasized that little is known about the Pt-Si in this semiconductor device and, therefore, unknown parameters must be introduced by guess, rather than fact. Specifically, for this calculation we require the free electron density in the Pt-Si region, and the density

of states effective mass of these free electrons. For the latter we assume (m^*/m) is equal to unity, which is indeed incorrect, but this parameter is unknown.

For the free electron density we have adjusted its magnitude to yield a reverse electric current typical of that obtained in experimental devices operating at 77° K. Our best guess is that the Pt-Si region contains a free electron density of approximately $10^{20} \text{ (cm}^{-3}\text{)}$, which implies this region is more accurately classified as a degenerate semiconductor, rather than a metal. Figure 27 illustrates the calculated reverse electric current vs. applied voltage, assuming a free electron density between $10^{20} \text{ (cm}^{-3}\text{)}$ and $1.5 \times 10^{20} \text{ (cm}^{-3}\text{)}$, assuming an energy barrier W_c of 0.27 (ev). Similarly, using conventional theoretical concepts the calculated reverse current is illustrated in Fig. 28; this calculated current is independent of the Pt-Si characteristics.

These calculations suggest that the reverse current of a p-type Pt-Si diode will be many orders of magnitude larger than predicted from traditional theoretical concepts. Further, implied by these calculations is that without good control over the fabrication processes poor reproducibility might be expected in Pt-Si devices. For example, our calculated reverse current, at a given biasing voltage, changes by nearly two orders of magnitude for a free electron density between $10^{20} \text{ (cm}^{-3}\text{)}$ and $1.5 \times 10^{20} \text{ (cm}^{-3}\text{)}$.

It can be shown that an assumed barrier W_c of 0.27 ev locates the valence band edge at the interface, E_b in Fig.1, below the conduction band edge, E_c . For this reason the mechanism of direct electron transition cannot take place between the valence band and the Pt-Si region of this device. Nonetheless, calculations show that the transition energy E_t lies close to the conduction band edge E_c yielding a true energy barrier of about $E_c - E_b$, rather than $E_f - E_b = 0.27 \text{ (ev)}$, as suggested by conventional theory. It is suggested that this significant difference between the assumed energy barrier and the true energy barrier produces the unexpected large reverse electric current in a Pt-Si diode.

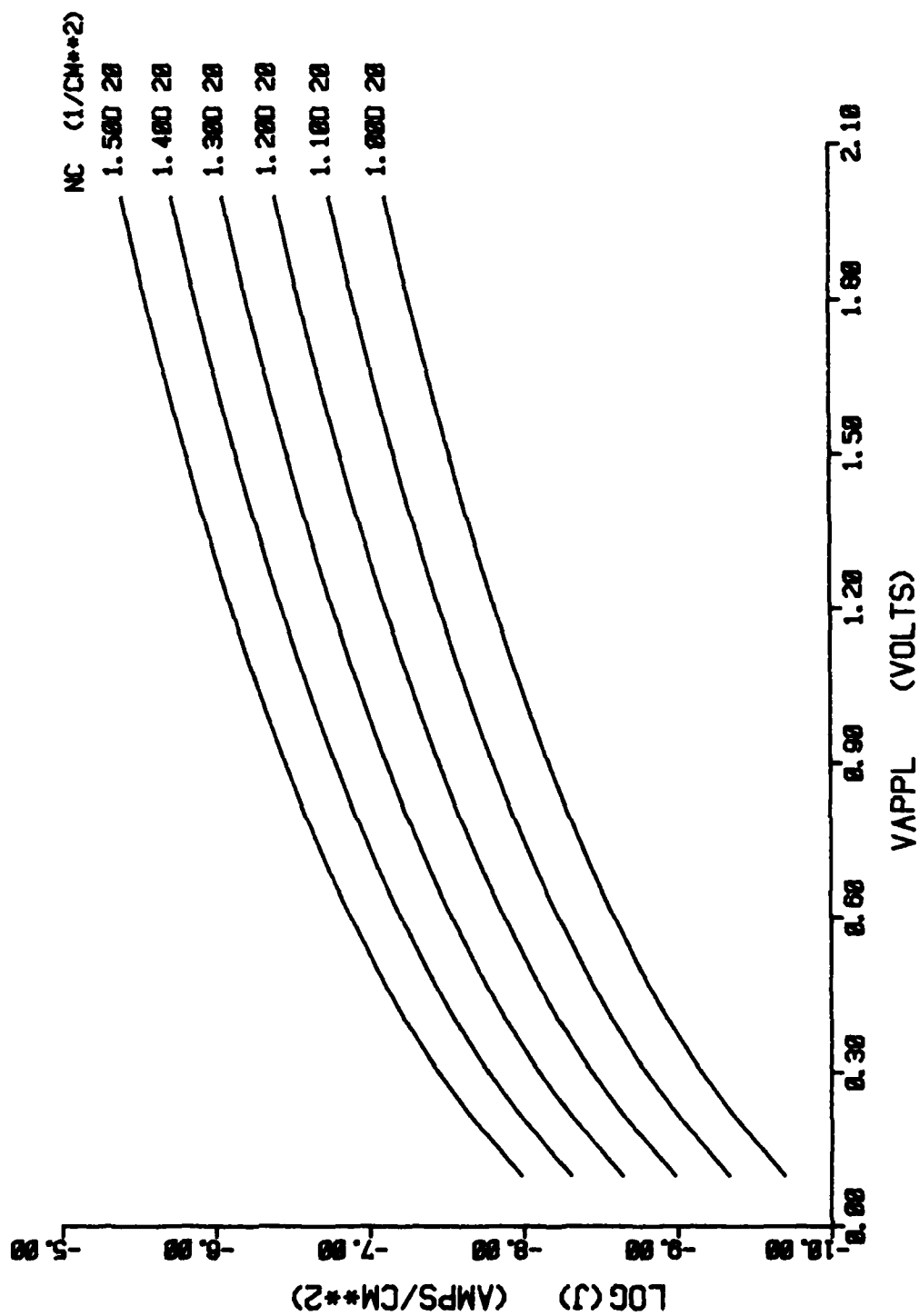


Fig. 27 Calculated Volt-Ampere Characteristics Based Upon Results from this Research
(Assumed Barrier $W_c = 0.27$ ev, $T = 77^\circ \text{K}$)

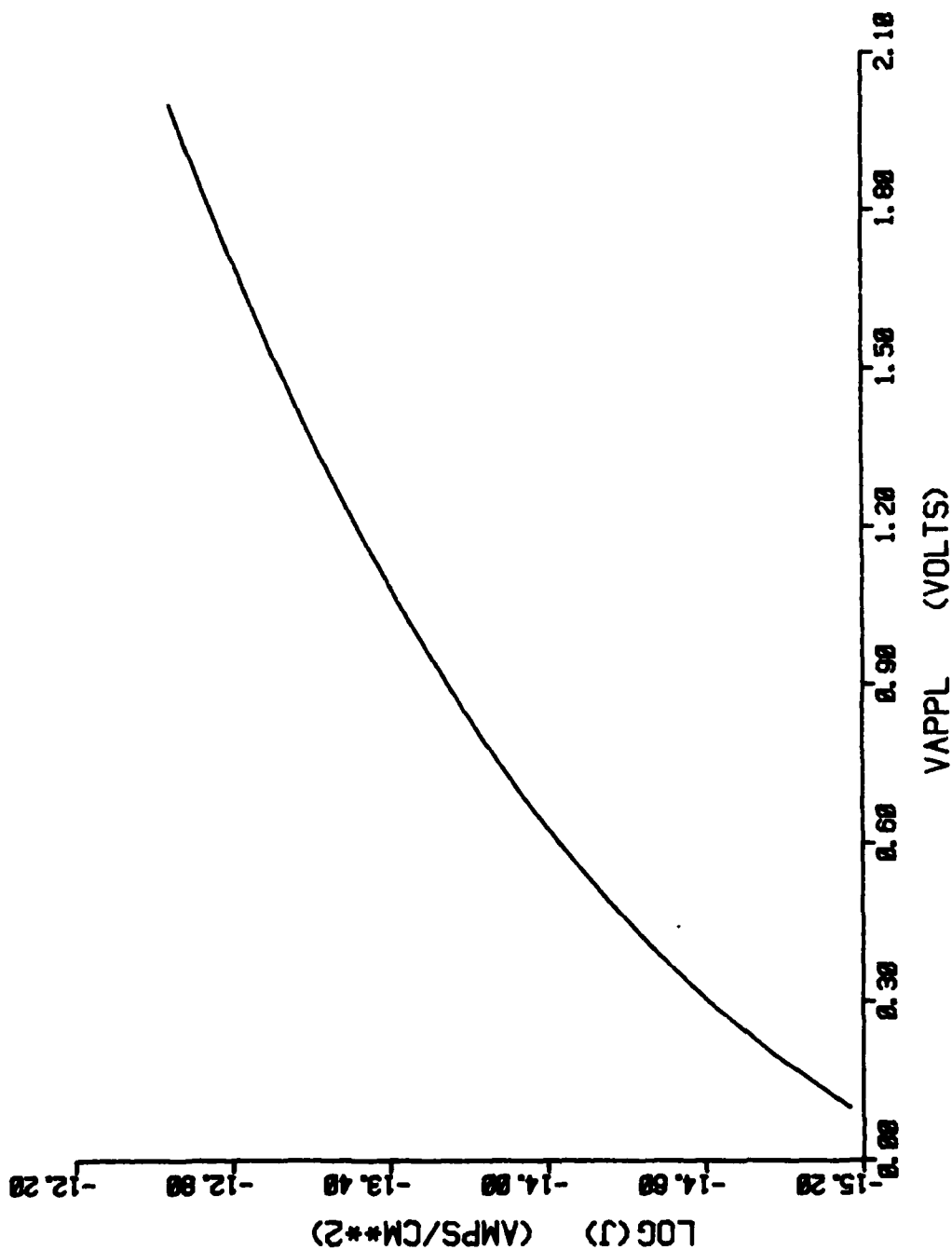


Fig.28 Calculated Volt-Ampere Characteristics of a Schottky Barrier Based upon Conventional Device Concepts (Assumed Barrier $W_c = 0.27$ ev, $T = 77^\circ$ K)

Chapter II

Potential Calculations for a Schottky Barrier Diode

1.0 Introduction

Most mathematical models of semiconductor device operation are based upon the concepts and mathematical equations outlined by W. Van Roosbroek [7] in 1950. In one spatial dimension, the steady-state form of these equations are given by:

$$\begin{aligned} \text{a)} \quad & \frac{d^2 \Psi}{dx^2} = - \frac{q}{k \epsilon_0} (N_D - N_A - n + p) \\ \text{b)} \quad & J_p = -q D_p \frac{dp}{dx} - q \mu_p p \frac{d\Psi}{dx} \\ \text{c)} \quad & J_n = q D_n \frac{dn}{dx} - q \mu_n n \frac{d\Psi}{dx} \quad (2-1) \\ \text{d)} \quad & \frac{dJ_p}{dx} = C_1 \\ \text{e)} \quad & \frac{dJ_n}{dx} = C_2 \\ \text{f)} \quad & J_T = J_p + J_n \end{aligned}$$

Equation (2-1a) is Poisson's equation, and it relates the divergence of the electric field to the electrostatic charge distribution arising from both mobile charge carriers (holes p and electrons n), and immobile ionized impurity atoms within the semiconductor lattice.

Equations (2-1b) and (2-1c) give the electric current density arising from the transport of mobile holes and electrons. These equations express the dependency of each electric current component, J_p and J_n , upon the concentration gradient of holes and electrons, the mobility of these charge carriers, and the electric field within the semiconductor material.

Equations (2-1d) and (2-1e) are the continuity equations for holes and electrons in a semiconductor, and these equations contain unspecified rates of carrier generation and recombination.

Equation (2-1f) states that the total electric current density, J_T , is the sum of the electric current due to holes, J_p , and electrons, J_n .

Throughout this analysis we assume the applicability of Boltzmann statistics, and the hole and electron densities are given by

$$\begin{aligned} \text{a)} \quad n &= n_i \exp - \left[q (\Psi - \phi_n) / kT \right] \\ \text{b)} \quad p &= n_i \exp - \left[q (\phi_p - \Psi) / kT \right] \end{aligned} \tag{2-2}$$

where ϕ_n and ϕ_p are the quasi-Fermi potentials for electrons and holes, respectively.

The carrier generation/recombination term in Eqs.(2-1d) and (2-1e) is assumed composed of three terms: first, carrier generation/recombination through defects, second by impact and/or avalanche ionization and, third, hole generation through valence electron transitions from the valence band of p-type silicon to the metal.

Hole/electron generation and recombination through defects are represented by a Hall-Schockley-Read (HSR) single level model [8,9] which characterizes defects with neutral and single charge states. Carrier generation/recombination through a single defect level center [10] is given by:

$$R = C \frac{pn - n_i^2}{n+p+2n_i \cosh \left[\frac{q(\phi_t - \phi_i)}{kT} \right]}, \quad (2-3)$$

where ϕ_t represents the trap potential and ϕ_i represents the intrinsic Fermi potential in silicon.

Calculations suggest that at the temperatures considered here (77° K-110° K) terms in Eqs.2-1 involving electrons in p-type silicon will have a negligible influence upon the results attained. For this reason such terms have been neglected and, thereby, these equations are reduced to the form

$$\begin{aligned} \text{a)} \quad & \frac{d^2 \psi}{dx^2} = \frac{q}{K \epsilon_0} (N_A - p) \\ \text{b)} \quad & J_p = -qD_p \frac{dp}{dx} - q\mu_p \frac{d\psi}{dx} \\ \text{c)} \quad & \frac{dJ_p}{dx} = \frac{dJ_n}{dx} = C \end{aligned} \quad (2-4)$$

2.0 Electric Current Continuity

Many investigations of diode operation neglect the influence of electric current upon the electrostatic potential distribution. Such a

simplification is achieved by maintaining constant the electron and hole quasi-Fermi potentials. In the presence of a large ionized impurity atom density little error results from this simplification, particularly when the reverse current is relatively small. Nonetheless, velocity limited carrier transport in a reverse biased diode does produce a significant amount of mobile carrier accumulation and, thereby, can modify the space-charge layer potential distribution.

For purposes of this analysis we attain electric current continuity by relating the divergence of electric current to the density of mobile carriers at a given location:

$$\frac{dJ_p}{dx} = R(p). \quad (2-5)$$

Both drift and diffusion mechanisms are assumed to contribute to the total electric current in Eq. 2-5 thus:

$$J_p = -qD_p \frac{dp}{dx} - q\mu_p p \frac{dp}{dx}. \quad (2-6)$$

3.0 Temperature Dependent Parameters

At low temperatures (77°K-110°K) many physical and electrical properties of silicon differ from that realized at room temperature. Unfortunately, substantial work remains to accurately characterize silicon at low temperature but, nonetheless, it is believed that many important low temperature material parameters are available in the technical literature.

a) Energy Gap

The energy gap E_g in silicon can be shown slightly temperature dependent^[11], and approximated by the relation:

$$E_g = 1.21 - 7.242 \times 10^{-3} (T/300) - 3.664 \times 10^{-2} (T/300)^2 \quad (2-7)$$

This expression represents an empirical fit to Fig.2-10 of Ref.11.

b) Intrinsic Fermi-Level

The intrinsic Fermi-level E_i is usually assumed located at the mid-gap of silicon. Nonetheless, in more rigorous calculations the intrinsic Fermi-level deviates slightly from this midgap position:

$$\begin{aligned} E_i - E_v &= E_g/2 + (k T/q) \ln (N_v/N_c) \\ &= E_g/2 - 1.206 \times 10^{-2} (T/300), \end{aligned} \quad (2-8)$$

where N_v and N_c represent the effective density of states at the valence and conduction band edges, respectively. In Eq.2-8 we assume $(N_v/N_c) = 1.02/2.8$, as stated in Ref.11, p.359.

c) Intrinsic Carrier Density

The intrinsic carrier density in silicon is exceedingly dependent upon the temperature, as shown in Ref.12, p.27:

$$n_i^2 = 4.9 \times 10^{15} (M_h^* M_e^* / M^2)^{3/4} T^{3/2} \exp(-E_g / 2 k T) \quad (2-9)$$

where M_h^* and M_e^* are the density of states effective mass for holes and electrons, respectively, and M is the free electron mass. This expression is approximated by

$$n_i = 3.925 \times 10^{19} (T/300)^{3/2} \exp(-E_g / 2 k T) \quad (2-10)$$

In Eq.2-10 the leading constants have been adjusted so that n_i equals $1.5 \times 10^{10} / \text{cm}^3$ when $T = 300^\circ \text{K}$.

d) Bulk Hole Density

In charge-neutral regions of p-type silicon the hole density is given by

$$p = n_i \exp (E_i - E_f) / k T \quad (2-11)$$

where n_i represents the intrinsic carrier density, E_i is the intrinsic Fermi-level, and E_f is the Fermi-level. Clearly, the hole density in charge neutral p-type silicon is exceedingly dependent upon the temperature.

e) Ionized Acceptor Density

The ionized acceptor density can be calculated using an expression of the form[13]:

$$N_I = \frac{N_A}{1 + \left[4 + 2 \exp (-q\Delta/k T) \right] \exp \left[-q(E_A - E_F) / k T \right]} \quad (2-12)$$

where $\Delta = .044$ ev; this term accounts for the spin orbit splitting at the valence band maximum in silicon.

f) Fermi-Level

Calculation of the Fermi-level E_F at a given temperature represents an iterative process. Specifically, at any given temperature T the Fermi-level must be such that charge neutrality exists in the material under consideration:

$$-N_A + p - n = 0. \quad (2-13)$$

In this calculation we ignore the electron density since at low temperatures this term has negligible influence upon Eq.2-13. Substituting Eq.2-10 into Eq.2-11 yields the hole

density in terms of the Fermi-level E_F . Thereafter, we substitute this expression and Eq.2-12 into Eq.2-13. We have the electrostatic charge in intrinsic silicon, as a function of the Fermi-level E_F . Thereafter the Fermi-level can be established using iterative methods to produce an electrostatic charge of zero.

Although the low-temperature mobility for holes is available in the technical literature[13], to date, this has not been implemented into this mathematical model.

4.0 Finite-Difference Implementation

Using traditional finite-difference techniques, this problem is solved on a one-dimensional grid containing a specified number of points (MAX = 100). These points are assumed equally spaced, and located between the ohmic contact to p-type silicon, and the metal-semiconductor interface.

In one spatial dimension, we designate a unit-cell of this one-dimensional array as composed of three locations: left, right, and center. Thereafter, applying central difference techniques in conjunction with the Taylor series, we can express the second derivative of electrostatic potential at this center location by the relation:

$$\left. \frac{d^2 \psi}{dx^2} \right|_c \approx \frac{\psi_l - 2\psi_c + \psi_r}{\Delta x^2}, \quad (2-14)$$

where Δx represents the distance between points on this array. Thereby, Poisson's equation in finite-difference form is given by

$$\frac{\psi_l - 2\psi_c + \psi_w}{\Delta x^2} = Q_c, \quad (2-15)$$

where Q_c is the electrostatic charge and is given by:

$$Q_c = \frac{q}{\kappa \epsilon_0} (N_A - p). \quad (2-16)$$

An equation similar to Eq. 2-16 can be written for each point on our approximating grid. When this is done we have 100 points and 100 equations, with 100 unknowns---the electrostatic potential at each location of the approximating grid.

Such a system of equations can be written in matrix form yielding a tri-diagonal matrix of rank 100. There is a multitude of different ways one can solve this matrix problem, each method yielding particular advantages and disadvantages.

A particular source of difficulty in finite-difference analysis is round-off error when solving large systems of equations. For this reason we have adopted the choleski decomposition technique [14-16], which has been found exceedingly stable in the presence of round-off error.

The choleski technique is based upon the fact that if a matrix B is positive definite, then B can be written as the product of a lower triangular matrix L and its transpose L^t thus

$$B = LL^t \quad (2-17)$$

and we have a two-step solution for this matrix problem.

It is emphasized that despite a direct solution for this matrix problem, solving Poisson's equation remains an iterative process. The exact mobile hole distribution is unknown and, therefore, iteration between the solution for $\psi(x)$ and $p(x)$ must continue until convergence is attained.

In an attempt to accelerate convergence of Poisson's equation we make use of Gummels algorithm [17]. This algorithm is based upon a linear approximation of the exponential relations appearing in the Boltzmann equa-

tion for holes, Eq.2-2b. We assume ψ^m , and p^m represent values of electrostatic potential and holes respectively, from m^{th} iteration step. Further, let $\psi^{m+1} = \psi^m + \delta^{m+1}$ where δ^{m+1} represents a small quantity. Thus, from the Boltzmann relation

$$\exp(\psi^{m+1}) = \exp(\psi^m) [1 + \delta^{m+1}] \quad (2-18)$$

thus

$$p^{m+1} = n^m (1 - \delta^{m+1}) \quad (2-19)$$

representing a prediction for the hole density at any location, resulting from the next iteration. Thereby, using Poisson's equation we have:

$$\frac{d^2 \psi^{m+1}}{dx^2} - \frac{q}{\kappa \epsilon_0} (p^m) \psi^{m+1} = \frac{q}{\kappa \epsilon_0} \left[N_A - p^m - p^m \psi^m \right]. \quad (2-20)$$

In finite difference form only the center terms need be modified: one term added to the finite difference element and a second term to the charge element.

In calculations of electric current continuity it is customary to employ similar finite-difference approximations to the expression for electric current, Eq.2-6, and substitute the results into an expression for the divergence of electric current. However, it can be shown that this procedure leads to numerical instability whenever the voltage difference between two mesh points exceeds about 5.1×10^{-2} volts [18]. Following Sharfetter and Gummel, the expression for electric current,

$$J_p = -qD_p \frac{dp}{dx} - q\mu_p p \frac{d\psi}{dx}, \quad (2-21)$$

is treated as a differential equation in p with J_p , μ_p and $d\psi/dx$ assumed constant between mesh points.

Thereby, we have a differential equation of the form

$$\frac{dp}{dx} + Ap + B = 0 \quad (2-22)$$

which can be solved between two finite-difference mesh points yielding

$$p_{n+1} = p_n \exp(U_{n+1} - U_n) - \frac{J \Delta x}{\mu (U_{n+1} - U_n)} \left[\exp(U_{n+1} - U_n) - 1 \right] \quad (2-23)$$

where U represents the normalized electrostatic potential ($U = q\psi / kT$).

Equation (2-23) relates the hole density at mesh point $n+1$ and n to the electric current between these mesh points. From Eq.(2-23) we can therefore write

$$J = \mu \frac{p_n \mu \Delta U}{\Delta x [\exp(\Delta U) - 1]} + \frac{p \mu \Delta U}{\Delta x [\exp(-\Delta U) - 1]} \quad (2-24)$$

where $\Delta U = U_{n+1} - U_n$. Equation (2-24) expresses the electric current between mesh points n and $n+1$ in terms of the potential and hole densities at these locations.

Designating the electric current into node n by J_w and out of node n by J_e , the divergence of electric current at node n is given by:

$$\frac{dJ_n}{dx} \approx \frac{J_e - J_w}{\Delta x} = C_n$$

where C represents the recombination/generation term assigned to node n . After substituting Eq.2-24 into Eq.2-25 for the east and west electric currents we obtain an expression for the divergence of electric current at each node in terms of the hole density at this node, and the two adjacent nodes.

Thereby we obtain a system of equations for the hole density---one equation for each node. This system represents a matrix equation for electron density that contains a sparse, tri-diagonal matrix. This system of equations is solved using the technique of Gauss elimination; by reducing the matrix to a triangular form and, thereafter, solving for the electron densities through backward substitution.

5.0 Boundary Conditions

Boundary conditions for this calculation are introduced in two different arrays: first, in the electrostatic potential array and, second, in the hole density array. Recognizing that all essential potential drop within a Schottky barrier device is encountered within the semiconductor material, this situation is introduced through an adjustment of the boundary conditions. Additionally, this mathematical model is directed toward an effective generation of holes at the metal-semiconductor interface; such a mechanism is also introduced through an adjustment of boundary conditions at this location.

For the solution of Poisson's equation we assume both end points of the one-dimensional array are maintained at a specified electrostatic potential: zero at the barrier interface, and at some positive applied voltage at the semiconductor ohmic contact. At each of these locations we have a finite-difference equation of the type:

$$A \psi_w + B \psi_c + D \psi_e = Q_c \quad (2-26)$$

If we designate the barrier interface at the western most location and the ohmic contact as the eastern most location, it is clear that A at the barrier and D at the ohmic contact do not, in fact, exist. Thus, setting

$$\text{(Barrier boundary)} \quad D = 0, \quad B = 1, \quad Q_c = (-N_A + p)$$

$$\text{(ohmic contact)} \quad A = 0, \quad B = 1, \quad Q_c = V_{\text{appl}}$$

The boundary conditions for the potential array are readily satisfied.

In the presence of an electric current the hole quasi-Fermi potential has some unspecified gradient distribution between the ohmic contact and the barrier interface. This gradient distribution is unknown, and it will depend upon the electric current density at each location within the device. If, indeed, the semiconductor ohmic contact lies far removed from the diode space-charge layer, the quasi-Fermi potential at that location will equal Fermi-potential, and at a point that is charge neutral. Further, if the hole Fermi-potential is maintained constant from the ohmic contact to the Schottky barrier we would model a device of this type in the absence of an electric current. Thus, reasonable boundary conditions appear to be attained by maintaining at the ohmic contact a hole quasi-Fermi potential equal to the Fermi-potential for the p-type semiconductor material. At the barrier interface we calculate the hole density using Eq.1-18, and thereby establish the quasi-Fermi potential at that location.

Thus, with knowledge of the quasi-Fermi potentials at the ohmic contact and at the barrier interface we can readily calculate the electron densities at these locations and, thereby, establish boundary conditions for solving the equation of electric current continuity.

6.0 Iterative Solution for the Schottky Barrier Diode

As previously discussed, iterative techniques are used to solve this problem of the Schottky barrier diode. A given solution is initiated by a first "guess" concerning the electrostatic potential and the hole density distributions. Thereafter, using iterative techniques, Poisson's equation is solved, and after each solution the hole distribution is updated, maintaining the initial guess for the hole quasi-Fermi potential; by recalculating the hole density we are establishing an improved solution for the electrostatic charge distribution.

Prior to each new calculation of the electrostatic charge in Poisson's equation, a determination is made concerning the degree of convergence. This is accomplished by calculating for each location of the potential array the expression:

$$A \psi_e + B \psi_c + D \psi_w - Q_c = R \quad (2-27)$$

which yields the error, or residual, at a given spatial location. Ideally, the true solution for this problem would yield a residual of zero everywhere.

Termination of this particular aspect of the calculation is attained when the maximum residual upon entry to the potential calculation is 10^{-4} (or less). Experience shows that any attempt at further refining the solution is of little practical value. In practice, this initial convergence of Poisson's equation is obtained with 100 (or less) iterations between electrostatic potential calculation and the hole density, for a given quasi-Fermi potential calculation.

After attaining convergence for this initial part of the potential calculation we obtain a very accurate solution for Poisson's equation, for our first guess about the quasi-Fermi potential distribution. Next, an improved solution for the quasi-Fermi potential is attained by solving the continuity equation for the hole density and recalculating a new quasi-Fermi potential.

After the initial convergence of Poisson's equation we no longer require the iteration between the electrostatic potential calculation and the hole density, maintaining the quasi-Fermi potential constant. After each new solution of Poisson's equation we immediately recalculate a new hole distribution and, hence, a new hole quasi-Fermi potential.

Final convergence for this system of equations is based upon simultaneously attaining three different convergence criterion:

1. When the starting residual is low prior to entry into the electrostatic potential calculation.
2. When the starting residual is low prior to entry into the calculation of electric current continuity.
3. When electric current continuity is attained within 1% of the total electric current.

From a practical point of view, excellent convergence is usually attained within 100 iterations between the solution of Poisson's equation and the solution for electric current continuity.

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APPENDIX 1

Computer Programs Developed During This Investigation

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A. Calculating Fermi Level vs. Temperature	83
B. Calculating Unoccupied States Between E_c and E_f	97
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Note: All computer programs listed in APPENDIX 1 are self contained.
The listings within a given function group can be keypunched,
compiled, linked, and run as a unit.

APPENDIX 1-A

Program for Calculating the Fermi-Level vs. Temperature

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MAIN	84
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XINT.	95

10.17 1981 9:50:51 FERMI.GV

COMPILE DOUBLE PRECISION

MAIN PROGRAM FOR CALCULATING THE FERMI LEVEL IN A CONDUCTOR
CONTAINING A SPECIFIED FREE ELECTRON DENSITY

USERSE:REQUIRES THE FOLLOWING SUBPROGRAMS:

FUNCTION EFERMI
SUBROUTINE ROOT
FUNCTION QUAD1
FUNCTION XINT

TEXP=EXPONENT FOR TEMP.

JMAX=TOTAL NUMBER OF ELECTRON DENSITY STEPS
EDLT=ELECTRON DENSITY STEP SIZE
EEXP=EXPONENT FOR ELECTRON DENSITY
KMAX=TOTAL NUMBER OF TEMP STEPS
TDLT=TEMP STEP SIZE
EMASS=ELECTRON MASS RATIO (M*/M)

LUOUT=CHANNEL FOR OUTPUT

ORIGINAL: D.P. KENNEDY & ASSOC. GAINESVILLE FLA.

DIMENSION DUMMY(10),A(50),B(50)
EXTERNAL EFERMI

-----INITIALIZE MISC CONSTANTS-----

EDLT=1.000
EEXP=2.001
KMAX=4
EMASS=1.000
TEXP=-2.5
TDLT=1.00-1

```

JMAX=13
LUOUT=10

-----TOP OF ELECTRON DENSITY STEPPING-----
DO 20 K=1,KMAX
  ELECT=1.001**EEXP
-----TOP OF TEMP STEPPING LOOP-----
  XEXP=TEXP
  DO 10 J=1,JMAX
    T=1.001**IXEXP
-----CALCULATE FERMI LEVEL AT ZERO K-----
    EF0=3.000*ELECT+1.20-21/(EMASS**((3.000/2.000)*6.814)
    EF0=EF0*(2.000/3.000)
    EF0=EF0/(8.6170-5*T)
-----CALCULATE FERMI LEVEL-----
    DUMMY(1)=EF0
    EF=EF0*0.7500
    EFMAX=1.002*EF0
    DELTE=EF0*5.00-1
    EPS=1.00-4

    CALL ROOT (EFERT,EF,EFMAX,DELTE,EPS,1,IER,DUMMY)
    IF(IER.NE.1) WRITE(LUOUT) 'ROOT NOT FOUND'
    IF(IER.NE.1) STOP

    WRITE(LUOUT,1111) TEXP,EF,EF0
1111 FORMAT(1X,' TEXP=',1P08.1,3X,' EF=',1P01.4,3X,' EF0=',1P01.4)
    XEXP=XEXP+TDLT
10 CONTINUE
END

```

10 / 17 / 1921

9 : 52 : 7

EFERMI.GV

FUNCTION EFERMI: IS USED TO CALC. THE FERMI LEVEL IN A
METALLIC CONDUCTOR

USAGE: REQUIRES SUBROUTINE QUAD1 AND FUNCTION XINT

ORIGINAL: D.P. KENNEDY, GAINESVILLE FLA.

FUNCTION EFERMI(EF,DUMMY)
DIMENSION DUMMY(10)
EXTERNAL XINT

-----INTEGRATE FROM 0 TO INF-----

```

EF0=DUMMY(1)
DUMMY(2)=EF
SUM=0.000
XX=EF-1.201
IF(XX.GT.0.000) SUM=2.010*(XX**((3.000/2.000)/3.000)
XUBND=0.000
IF(XX.GT.0.000) XUBND=XX
10 CONTINUE
XLBND=XUBND
XUBND=XUBND+1.001
XX=XUBND-EF
IF(XX.GT.1.002) GOTO 30
CALL QUAD1(XINT,XLBND,XUBND,RES,1/5,DUMMY)
SUM=SUM+RES
GOTO 10

```

```

30 CONTINUE
EFERMI=1.000-3.000*EF0+((-3.000/2.000)*SUM/2.000)

```

RETURN
END

10 17 1981 9 52 53 ROOT.GV

```

=====
SUBROUTINE 'ROOT' : LOCATES THE ROOT OF AN ARBITRARY FUNCTION
=====
USAGE : CALL ROOT (B,X,XMAX,DELX,EPS,IAR,IER,DUMMY)
WHERE : B,X,DUMMY = ARBITRARY FUNCTION
        DUMMY = A 10 ELEMENT ARRAY USED FOR PASSING
        PARAMETERS TO THE FUNCTION "B"
        X = MIN (MAX) VALUE OF X BEGINING SEARCH
        XMAX = MAX (MIN) VALUE OF X DURING SEARCH
        DELX = INITIAL STEP SIZE
              (+DELX INCREASES X , -DELX DECREASES X )
        EPS = PERMITTED FRACTIONAL ERROR
        IAR = ITERATION METHOD
              ( IAR = 0 BINARY CHOP )
              ( IAR = 1 METHOD OF SECANTS )
        IER = ERROR FLAG
              ( IER = 1 ROOT FOUND )
              ( IER = 0 ROOT NOT FOUND )

COMMENT : THE ROOT IS RETURNED THROUGH X . ALSO THE CALLING
PROGRAM MUST CLASSIFY THE FUNCTION NAME
TO BE PASSED THROUGH "B" AS EXTERNAL.
=====
ORIGINAL : APPLIED ELECTRONIC RESEARCH, GAINESVILLE, FLA. DEC. 1977
MOD#1 : AERC C.L. KENNEDY NOV. 1978
        IF X REACHES XMAX SET X=0 AND RETURN
=====

```

```

      1000000 : AERO D.P. KENNEDY NOV 1978
      1000000 : IMPROVED SEQR FLAG TER
      1000000 :
      1000000 : AERO D.P. KENNEDY NOV. 1978
      1000000 : SUBROUTINE CHANGE IN X
      1000000 : METHOD OF SECANTS INTRODUCED
      1000000 :
      1000000 : AERO C.L. KENNEDY DECEMBER 1978
      1000000 : ALL DUMMY VARIABLES PASSED
      1000000 : THROUGH ARRAY DUMMY
  
```

```

=====
  
```

```

SUBROUTINE ROOT (B,X,XMAX,DELX,EPS,IAP,TER,DUMMY)
  
```

```

      1000000 : IMPLICIT REAL*8(A-H,O-Z)
  
```

```

      1000000 : DIMENSION P(2),Q(2),DUMMY(1)
  
```

```

      1000000 : IF (DELX.EQ.0.000) GOTO 90
  
```

```

      1000000 : IER=1
  
```

```

      1000000 : P(1)=0.000
  
```

```

      1000000 : P(2)=0.000
  
```

```

      1000000 : Q(1)=0.000
  
```

```

      1000000 : Q(2)=0.000
  
```

```

      1000000 : Y=B(X,DUMMY)
  
```

```

      1000000 : P(1)=X
  
```

```

      1000000 : STEP TO BRACKET ROOT
  
```

```

      1000000 : X=X+DELX
  
```

```

      1000000 : P(2)=X
  
```

```

      1000000 : IF (DELX.GT.0.0.AND.X.GE.XMAX) GOTO 90
  
```

```

      1000000 : IF (DELX.LT.0.0.AND.X.LE.XMAX) GOTO 90
  
```

```

      1000000 : Z=B(X,DUMMY)
  
```

```

      1000000 : AB=(P(1)-P(2))/P(2)
  
```

```

      1000000 : IF (ABS(AB).LE.EPS) RETURN
  
```

```

      1000000 : A=Y#Z
  
```

```

      1000000 : P(1)=P(2)
  
```

```

IF (A.LT.0.000) GOTO 15
Y=Z
GOTO 10

```

```

-----
BINARY CHOICE METHOD OF SECANTS ?
-----

```

```

15 DEL=DELX
IF (IAR.EQ.1) GOTO 30

```

```

BINARY CHOICE

```

```

20 Y=Z
P(1)=P(2)
30 DEL=DEL/2.000
X=X-DEL
P(2)=X
Z=B(X,DUMMY)
AB=(P(1)-P(2))/P(2)
IF (DABS(AB).LE.EPS) RETURN
A=Y*Z
P(1)=P(2)
IF (A.LT.0.000) GOTO 40
GOTO 30

```

```

40 Y=Z
P(1)=P(2)
50 DEL=DEL/2.000
X=X+DEL
P(2)=X
Z=B(X,DUMMY)
AB=(P(1)-P(2))/P(2)
IF (DABS(AB).LE.EPS) RETURN
A=Y*Z
P(1)=P(2)
IF (A.LT.0.000) GOTO 20
GOTO 50

```

METHOD OF SECONDS

```

60 Q(2)=Z
P(2)=X
P(1)=X-DEL
PREP=R(1)
Q(1)=B(DUMMY,PREP)
70 XX=(P(2)*Q(1)-P(1)*Q(2))/(Q(1)-Q(2))
YY=B(XX,DUMMY)
P(1)=P(2)
Q(1)=Q(2)
P(2)=XX
Q(2)=YY
ERROR=DABS((P(1)-P(2))/P(2))
IF(ERROR.LE.EPS) GOTO 80
GOTO 70
80 X=XX
RETURN

```

```

ERROR RETURN Y=0 IER=0

```

```

90 X=0.000
IER=0
RETURN
END

```

10 / 17 / 1981 9 : 55 : 40 QUAD1.GV

=====

SUBROUTINE QUAD1: IS A QUADRATURE INTEGRATOR OF THE GAUSS-
LEGENDRE TYPE

=====

USAGE: CALL QUAD1(FUNC,XLBD,XURD,RES,IAR,DUMMY)
FUNC = FUNCTION TO BE INTEGRATED. THIS FUNCTION
MUST BE OF THE FORM FUNCTION FUNC(ARG,DUMMY)
DUMMY = 1-DIM DUMMY ARRAY FOR PASSING DATA
TO FUNC. THIS ARRAY MUST BE DIMENTIONED
IN THE CALLING PROGRAM.
XLBD = LOWER BOUND OF THE INTEGRAL
XURD = UPPER BOUND OF THE INTEGRAL
RES = RESULT
IAR = NUMBER OF TERMS IN THE INTEGRATION
(MAX=16,MIN=2)

NOTE: FUNC MUST BE CALLED OUT AS EXTERNAL BY THE
CALLING PROGRAM

REFERENCE:
NUMERICAL ANALYSIS. Z.KOPAL, CHAPTER VII,
CHAPMAN HALL, LONDON. 1961

=====

ORIGINAL: C.L. KENNEDY OCT. 1978
C.L. KENNEDY
MODN1-D.P. KENNEDY -- INTRODUCED GAUSS INTEGRATION FROM C
TO 16 TERMS SEPT 1981

SUBROUTINE QUAD1(FUNC,XLBD,XURD,RES,IAR,DUMMY)

COMMON /QUAD/ Z(8,16),U(8,16)

QUAD1.GV - 1

DIMENSION DUMMYY

C

DATA Z / 8*0.000.
 0.57335026318962600.7*0.000.
 0.77459563923149100.7*2.000.
 0.86113631159495200.0.33998104358485600.6*0.000.
 0.9061790473086400.0.5304693131956800.6*0.000.
 0.93246951420315200.0.66120938646626500.0.33861918000019100.5*0.100.
 0.94910791234225900.0.74153118559939400.0.4058451513739700.5*0.000.
 0.9502985649753600.0.7966647741362700.0.5255324090163200.
 0.1034346424956500.4*0.000.
 0.98016023950762600.0.83603110732663800.0.61337153270059000.
 0.3242532340380900.4*0.000.
 0.97390652851717200.0.8650633668898500.0.67043956829942400.
 0.43339539412924700.0.14887433898163100.3*0.000.
 0.97822865814605700.0.88706259976809500.0.73015200557404900.
 0.51909612920681200.0.26954315595234500.3*0.000.
 0.98156063424671900.0.90411725637047500.0.76990267419430500.
 0.5073179542866120.0.36783149999818000.0.12523340851146900.
 \$2*0.000.
 0.98418305471888000.0.91759839922297800.0.8015780907331000.
 0.64234933944034000.0.44849275103644700.0.23045831595513500.
 \$2*0.000.
 0.98628380809681200.0.92843488366357400.0.827220131506976500.
 0.68729290481168500.0.51524863635815400.0.31911236892789000.
 0.10005494870734400.0.000.
 0.98799251802048500.0.93727339240070600.0.84820658341042700.
 0.72441773136017000.0.57097217260853900.0.39415134707756300.
 0.20119409399743500.0.000.
 0.98940093499165000.0.94457592307323300.0.86567120238783200.
 0.7554040835500300.0.617876244026400.0.45801677765722700.
 0.20160355077925900.0.09501250983763700/
 DATA W / 8*0.000.
 \$1.000,7*0.000.
 0.55555555555555600.0.88888888888888900.6*0.000.
 0.34785484513745400.0.65214515486254600.6*0.000.
 0.23692688505618900.0.4786286704993600.0.56888888888888900.
 \$5*0.000.0.17132449237017000.0.36076157304813900.
 0.46791393457269100.5*0.000.0.12948496616887000.
 0.27970539148927700.0.381830050511900.0.41795919367346900.
 \$4*0.000.0.10122856329037600.0.22238107445337400.

C

```

00.31370664507780700.0.762663778377836200.
140.000.0.0012743936137400.0.1824813259425700.
12.2663169642029500.0.123477774422302.0.1703971530123000.
030.000.0.06667143300.0000.0.1495134915358100.
11.03933325159223.0.0692617933900600.0.295241271475100.
110.000.0.0556685571517400.0.1258033046492500.
10.1862821993773400.0.23319376459199300.
00.2609454451024700.0.27292580277790100.0.2111300.
00.24717533363651200.0.10693932599531800.0.1602032354334800.
00.2031674267306600.0.033492536530355200.0.2491479459140300.
120.000.0.0484840047631600.0.09212149983772800.
00.13987351021978700.0.17814599076194600.0.2270144753698400.
00.22620318022089700.0.03255155323087400.0.010.
10.03511946033175200.0.08015808715976000.0.12151257468790300.
00.15720315749219400.0.1855389747993800.0.20519846372122600.
00.21920385348315900.0.000.0.03075324199611700.
00.0723663474891800.0.1071592204677200.0.13957057792615400.
00.1662920581699400.0.18616100001556200.0.1984314853271200.
00.2025782419555100.0.0271524594175400.0.0602935239386800.
00.09515951168249300.0.12462897125553400.0.1495959881657700.
00.16915651939500300.0.02260341504492400.0.18945061445536800/

```

```

SUM=0.000
DO 10 I=1,8
IF(W(I,IAR).EQ.0) GOTO 10
ARG=(Z(I,IAR)+(XUBND-XLBND)+XUBND+XLBND)/2.000
TERM1=W(I,IAR)*FUNG(ARG,DUMMY)
ARG=(-Z(I,IAR)+(XUBND-XLBND)+XUBND+XLBND)/2.000
TERM2=0.000
IF(Z(I,IAR).NE.0.000) TERM2=W(I,IAR)*FUNG(ARG,DUMMY)
SUM=SUM+TERM1+TERM2
10 CONTINUE

RES=SUM*(XUBND-XLBND)/2.000

RETURN
END

```

QUAD1.GV - 3

95

APPENDIX I-B

Program for Calculating Unoccupied Energy States Between the Con-
duction Band Edge E_c and the Fermi-Level E_f

<u>Title</u>	<u>Page</u>
MAIN	98
XFERMI	101
EFERMI	103
ROOT	105
XINT	109
QUANDI	110
DIST	113


```

C      SEVP=0.001
C      EOLT=1.0D3
C      KMAX=4
C      EMASS=1.0D0
C      LUOUT=10
C      -----TOP OF ELECTRON DENSITY STEPPING LOOP-----
C      DO 40 N=1,KMAX
C      ELECT=1.0D1*EEXP
C      -----TOP OF TEMP STEPPING LOOP-----
C      XEXP=XEXP
C      DO 30 J=1,JMAX
C      T=1.0D1*(1-XEXP)
C      -----CALCULATE FERMI LEVEL-----
C      CALL XFERMI(ELECT,EFO.7,EMASS,EF,LUOUT)
C      -----INTEGRATE FROM EC TO EF-----
C      IEXIT=0
C      SUM=0.0D0
C      XUBND=0.0D0
C      25 CONTINUE
C      IF (IEXIT.EQ.1) GOTO 27
C      XLBND=XUBND
C      XUBND=XUBND+1.0D-2
C      IF (EF.GT.5.0D2) XUBND=XUBND+1.0D-3
C      IF (XUBND.GT.1.0D0) IEXIT=1
C      IF (IEXIT.EQ.1) XUBND=1.0D0
C      DUMMY(1)=EF
C      CALL QUADT(GOIST,XLBND,XUBND,RES.16,D MMY)
C      SUM=SUM+RES
C      GOTO 25
C      27 CONTINUE
C      XX=-3.0D0/2.0D0
C      ANS=3.0D0*((EF0/EF)+(XX))*SUM/2.0D0

```

```
WRITE(UNIT,ANS,'ANS  
A(1)=DLOG10(A(1))  
B(1)=XEXP  
XEXP=XEXP+0.112  
30 CONTINUE  
EEXP=EEXP+EEL  
40 CONTINUE  
END
```

10 1991 10 : 6 : 9 XFERM1.OV

COMPILE DOUBLE PRECISION

SUBROUTINE XFERM1 IS USED TO CALCULATE THE FERMI LEVEL
IN A METAL AT A SPECIFIED TEMP

USAGE: REQUIRES THE FOLLOWING
FUNCTION EFERMI
SUBROUTINE ROOT
FUNCTION XINT

ORIGINAL: D.P. KENNEDY & ASSOC., GAINESVILLE FLA.

SUBROUTINE XFERM1 (ELECT,EF0,T,EMASS,EF,LUOUT)

DIMENSION DUMMY(10),A(50),B(50)
EXTERNAL EFERMI

-----CALCULATE FERMI LEVEL AT ZERO K-----

EF0=3.00*ELECT*1.00-21/(EMASS*(3.00/2.00)*1.2368D1)
EF0=EF0*(2.00/3.00)
EF0=EF0/(8.617D-5*T)

-----CALCULATE FERMI LEVEL-----

DUMMY(1)=EF0
EF=EF0*0.7500
EFMAX=1.002*EF0
DELTE=EF0*5.00-1
EPS=1.00-4

XFERM1.OV 1

CALL ROOT (EFERMI,EF,EFMAX,DELTE,ES,1,IER,DUMMY)
IF IER.NE.1 WRITE(LUNOUT) ROOT NOT FOUND
IF (IER.NE.1) STOP
END

FUNCTION EFERR1 IS USED TO CALC. THE SEED LEVEL IN A
METALLIC CONDUCTOR

USAGE: REQUIRES SUPPORTING QUANT AND FUNCTION XINT

ORIGINAL: D.P. KENNEDY, CHINESEVILLE FLA.

FUNCTION EFERR1(DUMMY)
DIMENSION DUMMY(10)
EXTERNAL XINT

-----INTEGRATE FROM 0 TO INF-----

```

EF0=DUMMY(1)
DUMMY(2)=EF
SUM=0.000
XX=EF-1.000
IF (XX.GT.0.000) SUM=2.000*(XX+1.000)/2.000
XEND=0.000
IF (XX.GT.0.000) XEND=XX
10 CONTINUE
XEND=XEND+1.000
XX=XEND-EF
IF (XX.GT.1.000) GOTO 30
CALL QUANT(XINT,XEND,XEND.RES,16,DUMMY)
SUM=SUM+RES
GOTO 10

```

```

30 CONTINUE
EFERR1=1.000-3.000*EF0*(1-3.000/2.000)*SUM/2.000

```

AD-A113 211

KENNEDY (D P) AND ASSOCIATES INC GAINESVILLE FL
INVESTIGATION OF THE CURRENT VOLTAGE RELATIONSHIP FOR LOW BARRI-ETC(U)
FEB 82 D P KENNEDY

F/B 20/12

F19628-80-C-0020

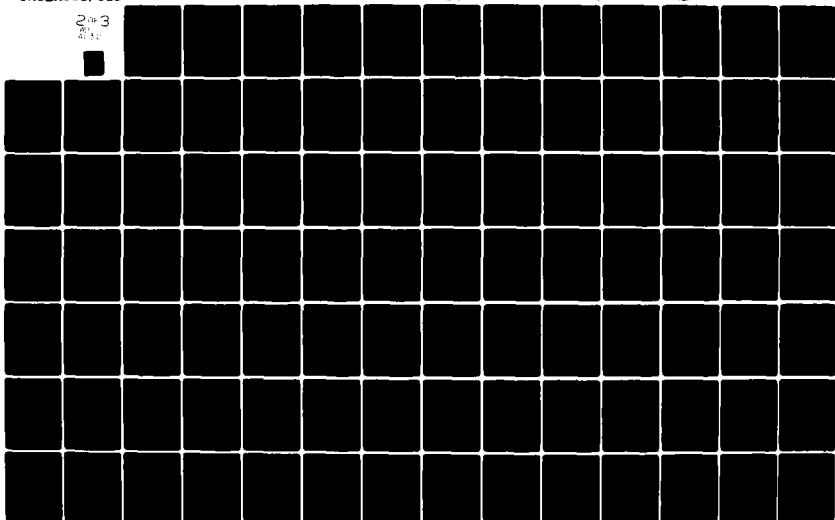
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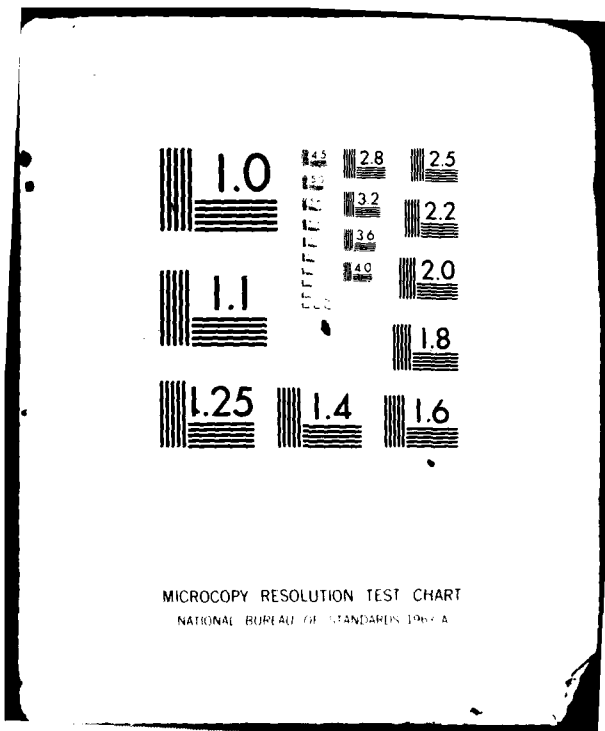
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RADC-TR-82-13

2 of 3

41 11





EFERNI.6V 2

RETURN
END

12 / 17 / 1981 10 : 7 : 44 ROOT.GV

SUBROUTINE ROOT : LOCATES THE ROOT OF AN ARBITRARY FUNCTION

USAGE : CALL ROOT (B,X,XMAX,DELX,EPS,IAR,IER,DUMMY)

WHERE : B(X,DUMMY) = ARBITRARY FUNCTION

DUMMY = A 10 ELEMENT ARRAY USED FOR PASSING
PARAMETERS TO THE FUNCTION "B"

X = MIN (MAX) VALUE OF X BEGINNING SEARCH

XMAX = MAX (MIN) VALUE OF X DURING SEARCH

DELX = INITIAL STEP SIZE

(+DELX INCREASES X , -DELX DECREASES X)

EPS = PERMITTED FRACTIONAL ERROR

IAR = ITERATION METHOD

(IAR = 0 BINARY CHOP)

(IAR = 1 METHOD OF SECANTS)

IER = ERROR FLAG

(IER = 1 ROOT FOUND)

(IER = 0 ROOT NOT FOUND)

COMMENT : THE ROOT IS RETURNED THROUGH X . ALSO THE CALLING
PROGRAM MUST CLASSIFY THE FUNCTION NAME
TO BE PASSED THROUGH "B" AS EXTERNAL.

ORIGINAL : APPLIED ELECTRONIC RESEARCH. GAINESVILLE. FLA. DEC. 1977

MOD#1 : AERC C.L. KENNEDY NOV. 1978

IF X REACHES XMAX SET X=0 AND RETURN

ROOT.GV -- 1

```

MOD#2 : AERC I.P. KENNEDY NOV 1978
      . INTRODUCED ERROR FLAG IER
MOD#3 : AERC D.P. KENNEDY NOV. 1978
      . EPS=FRACTIONAL CHANGE IN X
      . METHOD OF SECANTS INTRODUCED
MOD#4 : AERC C.L. KENNEDY DECEMBER 1978
      . ALL DUMMY VARIABLES PASSED
      . THROUGH ARRAY DUMMY
=====

```

```

SUBROUTINE ROOT (B,X,XMAX,DELX,EPS,IAR,IER,DUMMY)

```

```

      # IMPLICIT REAL*8(A-H,O-Z)

```

```

      DIMENSION P(2),Q(2),DUMMY(1)

```

```

      IF (DELX.EQ.0.000) GOTO 90

```

```

      IER=1

```

```

      P(1)=0.000

```

```

      P(2)=0.000

```

```

      Q(1)=0.000

```

```

      Q(2)=0.000

```

```

      Y=B(X,DUMMY)

```

```

      P(1)=X

```

```

-----
STEP TO BRACKET ROOT
-----

```

```

10 X=X+DELX

```

```

      P(2)=X

```

```

      IF (DELX.GT.0.0.AND.X.6E.XMAX) GOTO 90

```

```

      IF (DELX.LT.0.0.AND.X.LE.XMAX) GOTO 90

```

```

      Z=B(X,DUMMY)

```

```

      AB=(P(1)-P(2))/P(2)

```

```

      IF (DABS(AB).LE.EPS) RETURN

```

```

      A=Y#Z

```

```

      P(1)=P(2)

```

```

IF (A.LT.0.000) GOTO 15
Y=Z
GOTO 10

```

```

-----
BINARY CHOP OR METHOD OF SECANTS
-----

```

```

15 DEL=DELX
IF (AR.EQ.1) GOTO 60

```

```

BINARY CHOP
-----

```

```

20 Y=Z
P(1)=P(2)
30 DEL=DEL/2.000
X=X-DEL
P(2)=X
Z=B(X,DUMMY)
AB=(P(1)-P(2))/P(2)
IF (DABS(AB).LE.EPS) RETURN
A=Y*Z
P(1)=P(2)
IF (A.LT.0.000) GOTO 40
GOTO 30

```

```

40 Y=Z
P(1)=P(2)
50 DEL=DEL/2.000
X=X+DEL
P(2)=X
Z=B(X,DUMMY)
AB=(P(1)-P(2))/P(2)
IF (DABS(AB).LE.EPS) RETURN
A=Y*Z
P(1)=P(2)
IF (A.LT.0.000) GOTO 20
GOTO 50

```

C

METHOD OF SECANTS

```

50 Q(2)=Z
   P(2)=Y
   P(1)=X-DEL
   PREP=P(1)
   Q(1)=B(DUMMY,PREP)
70 XX=(P(2)*Q(1)-P(1)*Q(2))/(Q(1)-Q(2))
   YY=B(XX,DUMMY)
   P(1)=P(2)
   Q(1)=Q(2)
   P(2)=XX
   Q(2)=YY
   ERROR=DABS((P(1)-P(2))/P(2))
   IF(ERROR.LE.EPS) GOTO 80
   GOTO 70
80 X=XX
   RETURN

```

ERROR RETURN X=0 IER=0

```

90 X=0.000
   IER=0
   RETURN
   END

```

10 : 17 : 1981

10 : 10 : 32

XINT.GV

FUNCTION XINT(ARG,DUMMY)

=====

FUNCTION XINT REPRESENTS THE DISTRIBUTION FUNCTION FOR
OCCUPIED ENERGY STATES IN A METAL THAT
RESIDE ABOVE THE CONDUCTION BAND EDGE.
THIS DISTRIBUTION IS BASED UPON THE FERMI
-DIRAC DISTRIBUTION

=====

DIMENSION DUMPT(10)
EF=DUMMY(2)

A=DSORT(ARG)
B=ARG-EF
IF(B.GT.1.602) B=1.602
IF(B.LT.-1.602) B=-1.602
DENOM=1.000+DEXP(B)
XINT=A/DENOM

RETURN
END

XINT.GV - 1

10 * 12 * 1981 10 : 11 : 2 QUAD1.GV

=====

SUBROUTINE QUAD1 IS A QUADRATURE INTEGRATOR IN THE GAUSS-
 LEGENDE TYPE

=====

USAGE: CALL QUAD1(FUNC,XLBD,XUBND,RES,IAR,DUMMY)
 FUNC = FUNCTION TO BE INTEGRATED. THIS FUNCTION
 MUST BE OF THE FORM FUNCTION FUNC(ARG,DUMMY)
 DUMMY = 1-DIM DUMMY ARRAY FOR PASSING DATA
 TO FUNC. THIS ARRAY MUST BE DIMENTIONED
 IN THE CALLING PROGRAM.
 XLBD = LOWER BOUND OF THE INTEGRAL
 XUBND = UPPER BOUND OF THE INTEGRAL
 RES = RESULT
 IAR = NUMBER OF TERMS IN THE INTEGRATION
 (MAX=16,MIN=2)

NOTE:

FUNC MUST BE CALLED OUT AS EXTERNAL BY THE
 CALLING PROGRAM

REFERENCE:

NUMERICAL ANALYSIS, Z.KOPAL, CHAPTER VII,
 CHAPMAN HALL, LONDON, 1961

=====

OPTIONAL: C.L. KENNEDY OCT. 1978
 C.L. KENNEDY
 MODM1-D.P. KENNEDY --INTRODUCED GAUSS INTEGRATION FROM 2
 TO 16 TERMS SEPT 1981

SUBROUTINE QUAD1(FUNC,XLBD,XUBND,RES,IAR,DUMMY)

COMMON /QUAD/ Z(8,16),W(8,16)

11-SECTION DATA(1)

DATA 1 / 8*0.000,

1.5723502001806200,0.7*0.000,
 10.77499630024148300,7*0.000,
 11.32113631159495300,0.3399010435848500,6*0.000,
 11.9217984593866400,0.5384693101056800,6*0.000,
 11.93245951420315200,0.6612093864626000,0.23861918608319700,5*0.000,
 11.949107912342342900,0.74153118559939400,0.4058451513739700,5*0.000,
 11.95202985649753600,0.7966647741362700,0.52553248991632900,
 11.1333346424956500,4*0.000,
 11.93016023950732600,0.83603110732663600,0.61337143270059000,
 11.3125334340380900,4*0.000,
 11.9239255285177200,0.8650633668898500,0.67940956929982400,
 11.43339539412044700,0.14887433098163100,3*0.000,
 11.9232285814605700,0.88706259976809500,0.73015200557404900,
 11.5109961292681200,0.26950315595234500,3*0.000,
 11.98156063424671900,0.9041125637047500,0.76990267419430500,
 11.58731795428661700,0.36783149899818000,0.12523340851146900,
 12*0.000,
 11.99413335471358800,0.91759839922297800,0.80157809073331000,
 11.6243493394403400,0.4484275103644700,0.2304581595513500,
 12*0.000,
 11.9828380069681200,0.92843488366357400,0.82720131503976500,
 11.6872920481169500,0.51524863635815400,0.31911236892789000,
 11.1800549487073400,0.000,
 11.98799251802048500,0.93727339240070600,0.84820658341042700,
 11.72441723136017000,0.57097217240253900,0.3941513470756300,
 11.20119409399743500,0.000,
 11.98940093499145000,0.94457502307323300,0.86563120218783200,
 11.75540440835500300,0.6178762444026400,0.4580167765722700,
 11.28160355077925900,0.09501250903763700/

DATA 4 / 8*0.000,

11.002.7*0.000,
 11.55555555555555600,0.8888888888888900,6*0.000,
 11.34785484513745400,0.6521451548625400,6*0.000,
 11.23692488505618900,0.47862867049936600,0.56888888888889000,
 11.5*0.000,0.17132449237917000,0.36876157304813900,
 11.46791393457269100,5*0.000,0.12948486616887000,
 11.27970539148927700,0.381830050511900,0.11795918367346900,
 11*0.000,0.10122856329037600,0.2323810344537400,

```

$0.31370664587788700,0.0362887793370316300,
$4+0.000,0.000,27438836157460,0.18064811289485700,
$0.260106940293500,0.321472704002200,0.3302393550012100,
$0+0.000,0.066673443086800,0.14945134915058100,
$0.2188936051598200,0.26924271930009500,0.2955247211141500,
$3+0.000,0.0555668571017400,0.1255803016494500,
$0.18419021992773400,0.23319376459199300,
$0.05680454431024700,0.27293528677790150,2+0.000,
$0.04717533638651200,0.10693932599531800,0.1007830554334600,
$0.20316742072306000,0.23349253653935513,0.2491470458130320,
$2+0.000,0.0434800476531600,0.09212149983772800,
$0.13887351021978700,0.17814598076194600,0.2078160453638900,
$0.22628318026289700,0.2325515532087400,0.000,
$0.03511946033175200,0.08015808715976000,0.1215185768700300,
$0.15720316715819400,0.1855839747793800,0.20519848172120600,
$0.21526385346315800,0.000,0.23275321199611700,
$0.07836604748818000,0.10715922046717200,0.1395703702615400,
$0.16626920581699300,0.18616100001556200,0.19843148532711200,
$0.20557824192556100,0.02715245941175400,0.06222535239394800,
$0.09515851168249300,0.12432897125553400,0.14959598881657700,
$0.1615651939500300,0.18260341504492400,0.18945061045506800/

```

```

SUM=0.000
DO 10 I=1,8
  IF(W(I,IAR).EQ.0) GOTO 10
  ARG=(Z(I,IAR)*(XUBND-XLBND)+XUBND+XLBND)/2.000
  TERM1=W(I,IAR)*FUNC(ARG,DUMMY)
  ARG=(-Z(I,IAR)*(XUBND-XLBND)+XUBND+XLBND)/2.000
  TERM2=0.000
  IF(Z(I,IAR).NE.0.000) TERM2=W(I,IAR)*FUNC(ARG,DUMMY)
  SUM=SUM+TERM1+TERM2
10 CONTINUE
RES=SUM*(XUBND-XLBND)/2.000

```

```

RETURN
END

```

10 / 17 / 1981

12 : 14 : 9

DIST.BV

FUNCTION DIST(ARG,DUMMY)

=====

FUNCTION DIST: REPRESENTS THE DISTRIBUTION FUNCTION FOR
UNOCCUPIED ENERGY STATES IN A METAL THAT
RESIDE ABOVE THE CONDUCTION BAND EDGE.
THIS DISTRIBUTION IS BASED UPON THE FERMI
-DIRAC DISTRIBUTION

=====

DIMENSION DUMMY(10)
EFC=DUMMY(1)

A=DSQRT(ARG)
B=EFC*(1.000-ARG)
IF(B.GT.1.602) B=1.602
IF(B.LT.-1.602) B=-1.602
DENOM=1.000*DEXP(B)
DIST=A/DENOM

RETURN
END

APPENDIX 1-C

Program for Calculating Unoccupied Energy States Between the Fermi-Level E_f and an Energy E_b Where $(E_c < E_b < E_f)$

<u>Title</u>	<u>Page</u>
MAIN	116
QUADI	119
DIST	122
ROOT	123
XFERMI	127
EFERMI	129
XINT	131

[illegible]


```

WRITE(LUOUT,1111) EF,EF0,XEXP,ANS,RATIO
1111 FORMAT(1X,EF=,1PD12.5,3X,EF0=,1PD12.5,3X,XEXP=,1PD10.2,
3X,ANS=,1PD12.5,3X,EB/EF=,1PD9.2)
XEXP=XEXP+IDLTY
30 CONTINUE
WRITE(LUOUT)
RATIO=RATIO+RDLTY
40 CONTINUE
C
END

```

10 / 17 / 1991

10 : 30 : 18

QUAD01.GV

=====

SUBROUTINE QUAD1: IS A QUADRATURE INTEGRATOR OF THE GAUSS-
LEGENDRE TYPE

=====

USAGE: CALL QUAD1(FUNC,XLBD,XUBND,RES,IAR,DUMMY)

FUNC = FUNCTION TO BE INTEGRATED. THIS FUNCTION
MUST BE OF THE FORM FUNCTION FUNC(ARG,DUMMY)

DUMMY = 1-DIM DUMMY ARRAY FOR PASSING DATA
TO FUNC. THIS ARRAY MUST BE DIMENTIONED
IN THE CALLING PROGRAM.

XLBD = LOWER BOUND OF THE INTEGRAL

XUBND = UPPER BOUND OF THE INTEGRAL

RES = RESULT

IAR = NUMBER OF TERMS IN THE INTEGRATION
(MAX=16,MIN=2)

NOTE:

FUNC MUST BE CALLED OUT AS EXTERNAL BY THE
CALLING PROGRAM

REFERENCE:

NUMERICAL ANALYSIS, Z.KOPAL. CHAPTER VII,
CHAPMAN HALL, LONDON, 1961

=====

ORIGINAL: C.L. KENNEDY OCT. 1978

C.L. KENNEDY

MOD#1-D.P. KENNEDY --INTRODUCED GAUSS INTEGRATION FROM 2
TO 16 TERMS SEPT 1981

=====

SUBROUTINE QUAD1(FUNC,XLBD,XUBND,RES,IAR,DUMMY)

COMMON /QUAD/ Z(8,16),W(8,16)

DIMENSION DUMMY

DATA 2 0*0.000,
 3.5735026918962600,7*0.000,
 0.77459669224149300,7*0.000,
 0.86113631159405300,0.33998104358485600,6*0.000,
 0.90617984593866400,0.53846931010568300,6*0.000,
 0.9324695142315200,0.66120938646626500,0.33861918609319700,5*0.000,
 0.94910791234275900,0.74153118559939400,0.40584515137739700,5*0.000,
 0.96028985649753600,0.7966647741362700,0.52553240991632900,
 0.18343464249565000,4*0.000,
 0.96816023550762600,0.83603110732663600,0.61337143270059000,
 0.32425342340380900,4*0.000,
 0.97390655285171200,0.86505336688898500,0.67940956929922400,
 0.43339539412924700,0.14887433898163100,3*0.000,
 0.97822865814605700,0.88706259976809500,0.73015200557404900,
 0.51909612920681200,0.26954315595234500,3*0.000,
 0.98156063424671900,0.90411725637047500,0.76990267419430500,
 0.58731795428661700,0.36783149899818000,0.12523340851146900,
 0.2*0.000,
 0.98418305471858800,0.91759839922297800,0.8015789073331000,
 0.64234933944034000,0.44849275103644700,0.23045831595513500,
 0.2*0.000,
 0.9862838869681200,0.92843488366357400,0.82720131506976500,
 0.6872929481168500,0.5152486365815400,0.31911236892789000,
 0.10805494870734400,0.000,
 0.98799251802008500,0.937273392402070600,0.84820658341042700,
 0.7244173136017000,0.57097217260853900,0.3941514707756300,
 0.20119409399743500,0.000,
 0.98940093499165000,0.94457502307323300,0.86563130238783200,
 0.73540440835500300,0.6170762440264400,0.4580167765722700,
 0.28160355077925900,0.09501250903763700,

DATA 4 / 8*0.000,
 11.000,7*0.000,
 0.55555555555555600,0.88888888888888900,6*0.000,
 0.34785484513745400,0.65214515486254600,6*0.000,
 0.23692688505618900,0.47862867099936600,0.56888888888888900,
 0.5*0.000,0.17132449237917000,0.36076157304813900,
 0.4679139457269100,5*0.000,0.12948496616887000,
 0.27970539148927700,0.38183005050511900,0.41795918367346900,
 0.4*0.000,0.10122856329037600,0.22238103445337400,

```

$0.31370664587788700,0.362683780337636200,
$1.0.000,0.0012743931157450,0.10014813369425700,
$0.260159643293500,0.31234707724400300,0.33023975500126000,
$3*0.000,0.06667134430868800,0.14945134915058100,
$0.21988636251598200,0.26926671930999600,0.29552422471475300,
$3*0.000,0.35566856711617400,0.12558036946490500,
$0.1862902102773400,0.23319376459199000,
$0.26280454451024700,0.27292508677790100,2*0.000,
$0.04717533638651200,0.10693932599531800,0.16007831854334600,
$0.20316742672306600,0.23349253653835500,0.24914704581343300,
$2*0.000,0.04248488476531600,0.09212149983772800,
$0.13827351021978700,0.17814598076194600,0.20781604753683900,
$0.22628318026289700,0.23255155323087400,0.000,
$0.0351194603175200,0.08015808715976000,0.12151857068790300,
$0.15720316715819420,0.18553839747793800,0.20519848372129600,
$0.21526385346315800,0.000,0.03075324199611700,
$0.07036604748810800,0.10715922046717200,0.13957067792615400,
$0.16626920581699400,0.18616100001556200,0.19843148532711200,
$0.20227824192556100,0.02715245941175400,0.04225352393844800,
$0.09515851168249300,0.12462897125553400,0.14959598881657700,
$0.16915651939500300,0.18260341504492400,0.18945061045506800/

```

```

SUM=0.000
DO 10 I=1,8
IF (W(I,IAR).EQ.0) GO TO 10
ARG=(Z(I,IAR)+(XUBND-XLBNB)+(XUBND+XLBNB)/2.000
TERM1=W(I,IAR)+FUNC(ARG,DUMMY)
ARG=(-Z(I,IAR)+(XUBND-XLBNB)+(XUBND+XLBNB)/2.000
TERM2=0.000
IF (Z(I,IAR).NE.0.000) TERM2=W(I,IAR)+FUNC(ARG,DUMMY)
SUM=SUM+TERM1+TERM2
10 CONTINUE
RES=SUM+(XUBND-XLBNB)/2.000
RETURN
END

```

```

10 / 17 / 1981      10 : 33 : 26      DIST.GU

```

```

FUNCTION DIST(ARG,DUMMY)

```

```

=====

```

```

FUNCTION DIST:REPRESENTS THE DISTRIBUTION FUNCTION FOR
UNOCCUPIED ENERGY STATES IN A METAL THAT
RESIDE ABOVE THE CONDUCTION BAND EDGE.
THIS DISTRIBUTION IS BASED UPON THE FERMI
-DIRAC DISTRIBUTION

```

```

=====

```

```

DIMENSION DUMMY(10)
EFC=DUMMY(1)

```

```

A=DSORT(ARG)
B=EFC*(1.0D0-ARG)
IF(B.GT.1.6D2) B=1.6D2
IF(B.LT.-1.6D2) B=-1.6D2
DENOM=1.0D0+DEXP(B)
DIST=A/DENOM

```

```

RETURN
END

```

10 / 17 / 1981

12 : 33 : 56

ROOT.6"

```

=====
SUBROUTINE ROOT : LOCATES THE ROOT OF AN ARBITRARY FUNCTION
USAGE : CALL ROOT (B,X,XMAX,DELX,EPS,IAR,IER,DUMMY)
WHERE : B(X,DUMMY) = ARBITRARY FUNCTION
.
. DUMMY = A 10 ELEMENT ARRAY USED FOR PASSING
. PARAMETERS TO THE FUNCTION "B"
.
. X = MIN (MAX) VALUE OF X BEGINING SEARCH
.
. XMAX = MAX (MIN) VALUE OF X DURING SEARCH
.
. DELX = INITIAL STEP SIZE
. ( +DELX INCREASES X , -DELX DECREASES X )
.
. EPS = PERMITTED FRACTIONAL ERROR
.
. IAR = ITERATION METHOD
. ( IAR = 0 BINARY CHOP )
. ( IAR = 1 METHOD OF SECANTS )
.
. IER = ERROR FLAG
. ( IER = 1 ROOT FOUND )
. ( IER = 0 ROOT NOT FOUND )
.
COMMENT : THE ROOT IS RETURNED THROUGH X . ALSO THE CALLING
. PROGRAM MUST CLASSIFY THE FUNCTION NAME
. TO BE PASSED THROUGH "B" AS EXTERNAL.
=====
ORIGINAL : APPLIED ELECTRONIC RESEARCH, GAINESVILLE, FLA. DEC. 1977
MODM1 : AERC C.L. KENNEDY NOV. 1978
. IF X REACHES XMAX SET X=0 AND RETURN
.
=====

```



```

IF(A.LT.0.000) GOTO 15
Y=Z
GOTO 10

```

C
C
C
C
C

```

-----
BINARY CHOP OR METHOD OF SECANTS ?
-----

```

```

15 DEL=DELX
IF(IAR.EQ.1) GOTO 60

```

C
C
C
C
C

```

BINARY CHOP
-----

```

```

20 Y=Z
P(1)=P(2)
30 DEL=DEL/2.000
X=X-DEL
P(2)=X
Z=B(X,DUMMY)
AB=(P(1)-P(2))/P(2)
IF(DABS(AB).LE.EPS) RETURN
A=Y#Z
P(1)=P(2)
IF (A.LT.0.000) GOTO 40
GOTO 30

```

C

```

40 Y=Z
P(1)=P(2)
50 DEL=DEL/2.000
X=X+DEL
P(2)=X
Z=B(X,DUMMY)
AB=(P(1)-P(2))/P(2)
IF(DABS(AB).LE.EPS) RETURN
A=Y#Z
P(1)=P(2)
IF (A.LT.0.000) GOTO 20
GOTO 50

```

C
C

C METHOD OF SECANTS

C
C
C

```

60 Q(2)=Z
   P(2)=X
   P(1)=X-DEL
   PREP=P(1)
   Q(1)=B(DUMMY,PREP)
70 XX=(P(2)+Q(1)-P(1)*Q(2))/(Q(1)-Q(2))
   YY=B(XX,DUMMY)
   P(1)=P(2)
   Q(1)=Q(2)
   P(2)=XX
   Q(2)=YY
   ERROR=DABS((P(1)-P(2))/P(2))
   IF(ERROR.LE.EPS) GOTO 80
   GOTO 70
80 X=XX
   RETURN

```

C
C
C
C
C

ERROR RETURN X=0 IER=0

```

90 X=0.000
   IER=0
   RETURN
   END

```

```

10 / 17 / 1981      10 : 36 : 43      XFERNI.SV
=====
COMPILER DOUBLE PRECISION
=====
SUBROUTINE XFERNI IS USED TO CALCULATE THE FERNI LEVEL
      IN A METAL AT A SPECIFIED TEMP
=====
      USAGE: REQUIRES THE FOLLOWING
              FUNCTION EFERNI
              SUBROUTINE ROOT
              FUNCTION XINT
=====
      ORIGINAL: D.P. KENNEDY & ASSOC., GAINESVILLE FLA.
=====
SUBROUTINE XFERNI (ELECT,EF0,T,EMASS,EF,LUOUT)
=====
      DIMENSION DUMMY(10),A(50),B(50)
      EXTERNAL EFERNI
=====
      -----CALCULATE FERNI LEVEL AT ZERO K-----
      EF0=3.000*ELECT+1.00-21/(EMASS*(3.000/2.000)*1.236801)
      EF0=EF0*(2.000/3.000)
      EF0=EF0/(8.6170-5*T)
      -----CALCULATE FERNI LEVEL-----
      DUMMY(1)=EF0
      EF=EF0*0.7500
      EFMAX=1.002*EF0
      DELTE=EF0*5.00-1
      EPS=1.00-4
=====

```

```
CALL ROOT (EFORMI,EF,EFMAX,DELTE,EPS,I,IER,DUMMY)  
IF(IER.NE.1) WRITE(LUOUT) 'ROOT NOT FOUND'  
IF(IER.NE.1) STOP  
END
```

EFERMI.GV

10 : 37 : 32

10 / 17 / 1981

=====

FUNCTION EFERMI: IS USED TO CALC. THE FERMI LEVEL IN A
METALLIC CONDUCTOR

USAGE: REQUIRES SUBROUTINE QUAD1 AND FUNCTION XINT

=====

ORIGINAL: D.P. KENNEDY, GAINESVILLE FLA.

=====

FUNCTION EFERMI(EF,DUMMY)
DIMENSION DUMMY(10)
EXTERNAL XINT

-----INTEGRATE FROM 0 TO INF-----

```

EF0=DUMMY(1)
DUMMY(2)=EF
SUM=0.000
XX=EF-1.201
IF(XX.GT.0.000) SUM=2.000*(XX*(3.000/2.000))/3.000
XUBND=0.000
IF(XX.GT.0.000) XUBND=XX
10 CONTINUE
XLBND=XUBND
XUBND=XUBND+1.001
XX=XUBND-EF
IF(XX.GT.1.002) GOTO 30
CALL QUAD1(XINT,XLBND,XUBND,RES,16,DUMMY)
SUM=SUM+RES
GOTO 10

```

```

30 CONTINUE
EFERMI=1.000-3.000*EF0+(-3.000/2.000)*SUM/2.000

```

RETURN
END

10 / 17 / 1981 10 : 38 : 19 XINT.GV

FUNCTION XINT(ARG,DUMMY)

=====

FUNCTION XINT: REPRESENTS THE DISTRIBUTION FUNCTION FOR
OCCUPIED ENERGY STATES IN A METAL THAT
RESIDE ABOVE THE CONDUCTION BAND EDGE.
THIS DISTRIBUTION IS BASED UPON THE FERMI
-DIRAC DISTRIBUTION

=====

DIMENSION DUMMY(10)
EF=DUMMY(2)

A=DSORT(ARG)
B=ARG-EF
IF(B.GT.1.6D2) B=1.6D2
IF(B.LT.-1.6D2) B=-1.6D2
DENOM=1.0D0+DEXP(B)
XINT=A/DENOM

RETURN
END

APPENDIX 1-D

Program for Calculating Unoccupied Energy States Between the Con-
duction Band Edge E_c and an Energy E_b Where $(E_c < E_b < E_f)$

<u>Title</u>	<u>Page</u>
MAIN	134
QUADI	137
DIST	140
ROOT	141
EFERMI	145
XINT	147
XFERMI	148

[illegible]


```

WRITE(LUOUT,1111) EF,EF0,XEXP,ANS,RATIO
1111 READ(RAT1X,EF=.1PD12.5.3X,EF0=.1PD12.5.3X,XEXP=.1PD12.2.
3X,ANS=.1PD12.5.3X,ES/EF=.1PD9.2)
XEXP=XEXP+TDLT
30 CONTINUE
WRITE(LUOUT)
C
RATIO=RATIO+RDLT
40 CONTINUE
END

```


3

DATA 2 / 842.798

DATA 4 / 248 AND

```

$0.31372664587788700,0.1626837833783362200,
1478.000,0.00127438836157400,0.18064816084985700,
$0.26061689642935500,0.31234707704023300,0.33023935500126000,
312.000,0.36337134430888000,0.14945134915058100,
$0.21908636251598000,0.26926671930996000,0.29552103471475300,
330.000,0.05566856711617400,0.12558036946490500,
$1.18629821092773400,0.23319376459199000,
$0.26280454451024700,0.27292508677791200,2*0.000,
$0.04717533638651200,0.10693932592531800,0.1607832854334600,
$0.20316742672306600,0.23349253653835500,0.2494704581340300,
$2.000,0.04048409476531600,0.09212149983772800,
$0.13887351021978700,0.17614598076194600,0.20781604753688500,
$0.22628318026289700,0.23255155323087400,0.000,
$0.03511946033175200,0.08015808715976000,0.1215185063790300,
$0.15720316715919400,0.18553839747793800,0.20519846372129600,
$0.2152338534315800,0.000,0.03075324199611700,
$0.07036604748810800,0.10715922046717200,0.13957067792615400,
$0.16626920581699400,0.18616100001556200,0.19843148532711200,
$0.20257824192556100,0.02715245941175400,0.06225352373864800,
$0.0951585118249300,0.1246287125553400,0.14959598881657700,
$0.16915651937500300,0.182600341504492400,0.189450610455506800/

```

```

SUM=0.000
DO 10 I=1,8
IF(W(I,IAR).EQ.0) GOTO 10
ARG=(Z(I,IAR)*(XUBND-XLEND)+XUBND+XLEND)/2.000
TERM1=W(I,IAR)*FUNC(ARG,DUMMY)
ARG=(-Z(I,IAR)*(XUBND-XLEND)+XUBND+XLEND)/2.000
TERM2=0.000
IF(Z(I,IAR).NE.0.000) TERM2=W(I,IAR)*FUNC(ARG,DUMMY)
SUM=SUM+TERM1+TERM2
10 CONTINUE

RES=SUM*(XUBND-XLEND)/2.000

RETURN
END

```

C
C
C

10 / 17 / 1981 10 : 47 : 22 DIST.GV

FUNCTION DIST(ARG,DUMMY)

```
=====
FUNCTION DIST REPRESENTS THE DISTRIBUTION FUNCTION FOR
UNOCCUPIED ENERGY STATES IN A METAL THAT
RESIDE ABOVE THE CONDUCTION BAND EDGE.
THIS DISTRIBUTION IS BASED UPON THE FERMI
-DIRAC DISTRIBUTION
=====
```

```
=====
DIMENSION DUMMY(10)
EFC=DUMMY(1)
=====
```

```
A=DSQRT(ARG)
B=EFC*(1.000-ARG)
IF(B.GT.1.6D2) B=1.6D2
IF(B.LT.-1.6D2) B=-1.6D2
DENOM=1.000+DEXP(B)
DIST=A/DENOM
```

```
=====
RETURN
END
=====
```

10 / 17 1281

10 : 47 : 52

ROOT.60

SUBROUTINE ROOT : LOCATES THE ROOT OF AN ARBITRARY FUNCTION

USAGE : CALL ROOT (B,X,XMAX,DELX,EPS,IAR,IER,DUMMY)

WHERE : B(X,DUMMY) = ARBITRARY FUNCTION

DUMMY = A 10 ELEMENT ARRAY USED FOR PASSING
PARAMETERS TO THE FUNCTION "B"

X = MIN (MAX) VALUE OF X BEGINNING SEARCH

XMAX = MAX (MIN) VALUE OF X DURING SEARCH

DELX = INITIAL STEP SIZE
(+DELX INCREASES X , -DELX DECREASES X)

EPS = PERMITTED FRACTIONAL ERROR

IAR = ITERATION METHOD
(IAR = 0 BINARY CHOP)
(IAR = 1 METHOD OF SECANTS)

IER = ERROR FLAG
(IER = 1 ROOT FOUND)
(IER = 0 ROOT NOT FOUND)

COMMENT : THE ROOT IS RETURNED THROUGH X . ALSO THE CALLING
PROGRAM MUST CLASSIFY THE FUNCTION NAME
TO BE PASSED THROUGH "B" AS EXTERNAL.

ORIGINAL : APPLIED ELECTRONIC RESEARCH, GAINESVILLE, FLA. DEC. 1977

MOD#1 : AERC C.L. KENNEDY NOV. 1978
IF X REACHES XMAX SET X=0 AND RETURN


```

IF(A.LT.0.000) GOTO 15
Y=Z
GOTO 10

```

```

-----
P R I M A R Y   C H O P   O R   M E T H O D   O F   S E C A N T S ?
-----

```

```

15 DEL=DELX
IF(IAR.EQ.1) GOTO 60

```

```

-----
P R I M A R Y   C H O P
-----

```

```

20 Y=Z
P(1)=P(2)
30 DEL=DEL/2.000
X=X-DEL
P(2)=X
Z=B(X,DUMMY)
AB=(P(1)-P(2))/P(2)
IF(DABS(AB).LE.EPS) RETURN
A=Y*Z
P(1)=P(2)
IF (A.LT.0.000) GOTO 40
GOTO 30

```

```

40 Y=Z
P(1)=P(2)
50 DEL=DEL/2.000
X=X+DEL
P(2)=X
Z=B(X,DUMMY)
AB=(P(1)-P(2))/P(2)
IF(DABS(AB).LE.EPS) RETURN
A=Y*Z
P(1)=P(2)
IF (A.LT.0.000) GOTO 20
GOTO 50

```

METHOD OF SECANTS

C
C
C

```

60 P(1)=Z
P(2)=X
P(1)=X-DEL
PREP=P(1)
Q(1)=B(DUMMY,PREP)
70 XX=(P(2)+Q(1)-P(1)*Q(2))/(Q(1)-Q(2))
Y=B(X,DUMMY)
P(1)=P(2)
Q(1)=Q(2)
P(2)=XX
Q(2)=Y
ERROR=DABS((P(1)-P(2))/P(2))
IF(ERROR.LE.EPS) GOTO 80
GOTO 70
80 X=XX
RETURN

```

C
C
C
C
C

ERROR RETURN X=0 IER=0

```

90 X=0.000
IER=0
RETURN
END

```

12 17 1981 10 : 50 : 39 EFERMI.0V

```

=====
FUNCTION EFERMI: IS USED TO CALC. THE FERMI LEVEL IN A
METALLIC CONDUCTOR
=====
USAGE:  REQUIRES SUBROUTINE QUAD1 AND FUNCTION XINT
=====
ORIGINAL:  R.F. KENNEDY, GAINESVILLE FLA.
=====
FUNCTION EFERMI(EF,DUMMY)
  DIMENSION DUMMY(10)
  EXTERNAL XINT
  -----INTEGRATE FROM 0 TO INF-----
  EFO=DUMMY(1)
  DUMMY(2)=EF
  SUM=0.000
  XX=EF-1.201
  IF (XX.GT.0.000) SUM=2.000*(XX**2+(3.000/2.000))/3.000
  XUBND=0.000
  IF (XX.GT.0.000) XUBND=XX
  10 CONTINUE
  XLBND=XUBND
  XUBND=XUBND+1.001
  XX=XUBND-EF
  IF (XX.GT.1.002) GOTO 30
  CALL QUAD1(XINT,XLBND,XUBND,RES,16,DUMMY)
  SUM=SUM+RES
  GOTO 10
  30 CONTINUE
  EFERMI=1.000-3.000*EFO+(-3.000/2.000)*SUM/2.000
=====

```

RETURN
END

```

10 / 17 / 199*      10 : 51 : 25      XINT.BY
=====
FUNCTION XINT(ARG,DUMMY)
=====
      FUNCTION XINT:REPRESENTS THE DISTRIBUTION FUNCTION FOR
      OCCUPIED ENERGY STATES IN A METAL THAT
      RESIDE ABOVE THE CONDUCTION BAND EDGE.
      THIS DISTRIBUTION IS BASED UPON THE FERMI
      -DIRAC DISTRIBUTION
=====
      DIMENSION DUMMY(10)
      EF=DUMMY(2)

      A=DSORT(ARG)
      B=ARG-EF
      IF(B.GT.1.6D2) B=1.6D2
      IF(B.LT.-1.6D2) B=-1.6D2
      DENOM=1./DD+DEXP(B)
      XINT=A/DENOM
=====
      RETURN
      END
=====

```

12 1 1981 12 1 51 55 XFERN1.G9

COMPILER DOUBLE PRECISION

=====

SUBROUTINE XFERN1 IS USED TO CALCULATE THE FERMI LEVEL
IN A METAL AT A SPECIFIED TEMP

=====

USAGE: REQUIRES THE FOLLOWING
FUNCTION EFERN1
SUBROUTINE ROOT
FUNCTION XINT

=====

ORIGINAL: D.P. KENNEDY & ASSOC., GAINESVILLE FLA.

=====

SUBROUTINE XFERN1 (ELECT,EF0,T,EMASS,EF,LUOUT)

DIMENSION DUMMY(10),A(50),B(50)
EXTERNAL EFERN1

-----CALCULATE FERMI LEVEL AT ZERO K-----

EF0=3.00*ELECT+1.00-21/(EMASS*(3.000/2.000)*1.236801)
EF0=EF0*(2.000/3.000)
EF0=EF0/(8.6170-5*T)

-----CALCULATE FERMI LEVEL-----

DUMMY(1)=EF0
EF=EF0*0.7500
EFMAX=1.002*EF0
DELTE=EF0*5.00-1
EPS=1.00-4

```
CALL ROOT (EFERMI,EF,EFMAX,DELTE,EPS,1,IER,DUMMY)
IF (IER.NE.1) WRITE(LUGUT) 'ROOT NOT FOUND'
IF (IER.NE.1) STOP
END
```

APPENDIX 1-E

Program for Calculating the Transition Energy W_t in a Metal-Semiconductor Contact.

<u>Title</u>	<u>Page</u>
MAIN	152
ROOT	156
DIST	160
ZERO	161
XFERMI	163
EFERMI	165
QUADI	167
XINT	170


```

XUBND=1.0D0-1.0D2/XX
IF(XUBND.LT.0.0D0) XUBND=0.0D0
EC=SEF#
25 CONTINUE
IF(IEIT.EQ.1) GOTO 27
XLBND=XUBND
XUBND=XUBND+1.0D1/XX
IF(XUBND.GT.EC/XX) IEIT=1
IF(IEIT.EQ.1) XUBND=EC/XX
DUMMY(1)=XX
CALL QUAD1(DIST,XLBND,XUBND,RES,16,DUMMY)
SUM=SUM+RES
IF(SUM.LT.1.0D-60) SUM=1.0D-60
GOTO 25
C
27 CONTINUE
YY=3.0D0/2.0D0
XNV=DLOG(3.0D0/2.0D0)+DLOG(VELECT)-YY*DLOG(SEF#/XX)
XNV=XNV+DLOG(SUM)
IF(XNV.LT.-1.6D2) XNV=-1.6D2
XNV=DEXP(XNV)
P=SEF#+BOLTZ*T
WRITE(10,1122) P,XNV
1122 FORMAT(1X,'SEF#=',1PD11.4,3X,'XNV=',1PD11.4)
C
C
C -----CALC.ET-----
DUMMY(1)=FELECT
DUMMY(2)=RATIO
DUMMY(3)=EF
DUMMY(4)=XMASS
DUMMY(5)=EFO
DUMMY(6)=XNV
DUMMY(7)=T
C
ARG=EF*RATIO
IF(ARG.LT.0.0D0) ARG=0.0D0
XX=ZERO(ARG,DUMMY)
IF(XX.GE.0.0D0) ET=ARG
IF(XX.GE.0.0D0) GOTO 5
C
ET=0.0D0
C

```

```

ETMAX=1.0D2*EF
DLTE=EF/10.0D0
EPS=1.0D-4

C
CALL ROOT(ZERO,ET,ETMAX,DLTE,EPS,0,IER,DUMMY)
IF(IER.NE.1) WRITE(LUOUT) 'ROOT FOR ET NOT FOUND'
IF(IER.NE.1) STOP

C
5 CONTINUE

C
EB=RATIO*EF
WT=(ET-EF)*RATIO*.8012+T
A(I)=WT
B(J)=XEXP
WRITE(LUOUT,111) EF,EF0,XEXP,ET,EB,WT
111 FORMAT(1X,'EF=',1P012.5,3X,'EF0=',1P012.5,3X,'TEMP=',1P010.2,
83X,'ET=',1P012.5,3X,'EB=',1P012.5,3X,'WT=',1P012.5)
XEXP=XEXP.TDLT
30 CONTINUE
WRITE(LUOUT)

C
WC=WC+VOLT
40 CONTINUE
END

```

10 / 17 / 1981

10 : 57 : 18

ROOT.F.GN

```

=====
SUBROUTINE ROOT : LOCATES THE ROOT OF AN ARBITRARY FUNCTION
USAGE : CALL ROOT (B,X,XMAX,DELX,EPS,IAR,IER,DUMMY)
WHERE : B(X,DUMMY) = ARBITRARY FUNCTION
.      DUMMY      = A 10 ELEMENT ARRAY USED FOR PASSING
.                PARAMETERS TO THE FUNCTION "B"
.      X          = MIN (MAX) VALUE OF X BEGINING SEARCH
.      XMAX       = MAX (MIN) VALUE OF X DURING SEARCH
.      DELX       = INITIAL STEP SIZE
.                ( +DELX INCREASES X , -DELX DECREASES X )
.      EPS        = PERMITTED FRACTIONAL ERROR
.      IAR        = ITERATION METHOD
.                ( IAR = 0 BINARY CHOP )
.                ( IAR = 1 METHOD OF SECANTS )
.      IER        = ERROR FLAG
.                ( IER = 1 ROOT FOUND )
.                ( IER = 0 ROOT NOT FOUND )

COMMENT : THE ROOT IS RETURNED THROUGH X . ALSO THE CALLING
.         PROGRAM MUST CLASSIFY THE FUNCTION NAME
.         TO BE PASSED THROUGH "B" AS EXTERNAL.
=====
ORIGINAL : APPLIED ELECTRONIC RESEARCH, GAINESVILLE, FLA. DEC. 1977
MOD#1   : AERC C.L. KENNEDY NOV. 1978
.         IF X REACHES XMAX SET X=0 AND RETURN
=====

```

```

C C C
MODR2 : AERE D.P. KENNEDY NOV 1978
      . INTRODUCED ERROR FLAG IER
C C C
MODR3 : AERE D.P. KENNEDY NOV. 1978
      . EPS=FRACTIONAL CHANGE IN X
      . METHOD OF SECANTS INTRODUCED
C C C
MODR4 : AERE C.L. KENNEDY DECEMBER 1978
      . ALL DUMMY VARIABLES PASSED
      . THROUGH ARRAY DUMMY
C C C
=====
SUBROUTINE ROOT (B,X,XMAX,DELX,EPS,IAR,IER,DUMMY)
C C C
      * IMPLICIT REAL*8(A-H,O-Z)
C C C
      DIMENSION P(2),Q(2),DUMMY(1)
C C C
      IF (DELX.EQ.0.000) GOTO 90
      IER=1
      P(1)=0.000
      P(2)=0.000
      Q(1)=0.000
      Q(2)=0.000
      Y=B(X,DUMMY)
      P(1)=X
C C C
      STEP TO BRACKET ROOT
C C C
      10 X=X+DELX
      P(2)=X
      IF (DELX.GT.0.0.AND.X.GE.XMAX) GOTO 90
      IF (DELX.LT.0.0.AND.X.LE.XMAX) GOTO 90
      Z=B(X,DUMMY)
      AB=(P(1)-P(2))/P(2)
      IF (DABS(AB).LE.EPS) RETURN
      A=Y+Z
      P(1)=P(2)

```

```

IF(A.LT.0.000) GOTO 15
Y=Z
GOTO 10

```

C
C
C
C
C

```

-----
BINARY CHOP OR METHOD OF SECANTS ?
-----

```

```

15 DEL=DELX
IF(IAR.EQ.1) GOTO 60

```

C
C
C
C
C

```

BINARY CHOP
-----

```

```

20 Y=Z
P(1)=P(2)
30 DEL=DEL/2.000
X=X-DEL
P(2)=X
Z=B(X,DUMMY)
AB=(P(1)-P(2))/P(2)
IF(DABS(AB).LE.EPS) RETURN
A=Y+Z
P(1)=P(2)
IF (A.LT.0.000) GOTO 40
GOTO 30

```

C

```

40 Y=Z
P(1)=P(2)
50 DEL=DEL/2.000
X=X+DEL
P(2)=X
Z=B(X,DUMMY)
AB=(P(1)-P(2))/P(2)
IF(DABS(AB).LE.EPS) RETURN
A=Y+Z
P(1)=P(2)
IF (A.LT.0.000) GOTO 20
GOTO 50

```

C
C

METHOD OF SECANTS

```

60 Q(2)=Z
   P(2)=X
   P(1)=X-DEL
   PREP=P(1)
   Q(1)=B(DUMMY,PREP)
70 XX=(P(2)*Q(1)-P(1)*Q(2))/(Q(1)-Q(2))
   YY=B(XX,DUMMY)
   P(1)=P(2)
   Q(1)=Q(2)
   P(2)=XX
   Q(2)=YY
   ERROR=DABS((P(1)-P(2))/P(2))
   IF(ERROR.LE.EPS) GOTO 80
   GOTO 70
80 X=XX
   RETURN

```

```

-----
ERROR RETURN X=0 IER=0
-----

```

```

90 X=0.000
   IER=0
   RETURN
END

```

12 / 17 / 1981

11 : 0 : 4

DIST.GV

FUNCTION DIST ARG.DUMMY)

=====

FUNCTION DIST: REPRESENTS THE DISTRIBUTION FUNCTION FOR
UNOCCUPIED ENERGY STATES IN A METAL THAT
RESIDE ABOVE THE CONDUCTION BAND EDGE.
THIS DISTRIBUTION IS BASED UPON THE FERMI
-DIRAC DISTRIBUTION

=====

DIMENSION DUMMY(10)
EFC=DUMMY(1)

A=DSORT(ARG)
B=EFC*(1.000-ARG)
IF(B.GT.1.602) B=1.602
IF(B.LT.-1.602) B=-1.602
DENOM=1.000+DEXP(B)
DIST=A/DENOM

RETURN
END

10 - 17 / 1981

11 : 0 : 34

ZERO.00

=====

FUNCTION ZERO: CALCULATES WITHIN AN ENERGY RANGE E AND
(E+DE) THE DIFFERENCE BETWEEN UNOCCUPIED
STATES IN THE METAL AND ELECTRONS WITH
A MAXWELLIAN DISTRIBUTION THAT ARE
AVAILABLE TO OCCUPY THESE STATES

=====

ORIGINAL: D.P. KENNEDY & ASSOC. GAINESVILLE, FLA.

=====

FUNCTION ZERO(ARG,DUMMY)
DIMENSION DUMMY(10)
FELECT=DUMMY(1)
EF=DUMMY(3)
XNV=DUMMY(6)
T=DUMMY(7)
BOLTZ=8.616600
PI=3.14159265

XX=ARG
IF(DABS(XX).LE.1.00-70) XX=1.00-70
TERM1=DLOG(3.000)+DLOG(FELECT)-3.000+DLOG(EF0)/2.000+DLOG(XX)
XX=EF-ARG
IF(XX.GT.1.502) TERM1=TERM1-XX
IF(XX.GT.1.502) GOTO 10
IF(XX.LT.-1.502) GOTO 10
TERM1=TERM1-DLOG(1.000+DEXP(XX))
10 CONTINUE

TERM2=-DLOG(DSORT(1.000/(2.000+PI*BOLTZ*T)))+DLOG(XNV)
XX=ARG-RATIO*EF
TERM2=TERM2-XX
ZERO=TERM1-TERM2

RETURN
END

10 / 17 / 1981 11 : 1 : 25 XFERMI.BV

COMPILER DOUBLE PRECISION

SUBROUTINE XFERMI IS USED TO CALCULATE THE FERMI LEVEL
IN A METAL AT A SPECIFIED TEMP

USAGE: REQUIRES THE FOLLOWING
FUNCTION EFERMI
SUBROUTINE ROOT
FUNCTION XINT

ORIGINAL: D.P. KENNEDY & ASSOC.. GAINESVILLE FLA.

SUBROUTINE XFERMI (ELECT,EF0,T,EMASS,EF,LUOUT)

DIMENSION DUMMY(10),A(50),B(50)
EXTERNAL EFERMI

-----CALCULATE FERMI LEVEL AT ZERO K-----

EF0=3.000+ELECT*1.0D-21/(EMASS*(3.000/2.000)+1.2368D1)
EF0=EF0*(2.000/3.000)
EF0=EF0/(8.617D-5+T)

-----CALCULATE FERMI LEVEL-----

DUMMY(1)=EF0
EF=EF0*0.7500
EFMAX=1.002*EF0
DELTE=EF0*5.00D-1
EPS=1.00D-4

```
CALL ROOT (EFERMI,EF,EFMAX,DELTE,EPS,,IER,DUMMY)  
IF (IER.NE.1) WRITE (LUOUT) 'ROOT NOT FOUND'  
IF (IER.NE.1) STOP  
END
```

EFERMI.GV

11 : 2 : 15

10 / 17 / 1981

```

=====
FUNCTION EFERMI: IS USED TO CALC. THE FERM. LEVEL IN A
      METALLIC CONDUCTOR
=====
USAGE:  REQUIRES SUBROUTINE QUAD1 AND FUNCTION XINT
=====
ORIGINAL: D.P. KENNEDY, GAINESVILLE FLA.
=====

FUNCTION EFERMI(EF,DUMMY)
  DIMENSION DUMMY(10)
  EXTERNAL XINT
  -----INTEGRATE FROM 0 TO INF-----

  EF0=DUMMY(1)
  DUMMY(2)=EF
  SUM=0.000
  XX=EF-1.201
  IF (XX.GT.0.000) SUM=2.000*(XX**((3.000/2.000)/3.000)
  XUBND=0.000
  IF (XX.GT.0.002) XUBND=XX
  10 CONTINUE
  XLBND=XUBND
  XUBND=XUBND+1.001
  XX=XUBND-EF
  IF (XX.GT.1.002) GOTO 30
  CALL QUAD1(XINT,XLBND,XUBND,RES,16,DUMMY)
  SUM=SUM+RES
  GOTO 10

  30 CONTINUE
  EFERMI=1.000-3.000*EF0**(-3.000/2.000)*SUM/2.000

```

RETURN
END

10 / 17 / 1981

11 : 3 : 1

QUAD1.GV

=====

SUBROUTINE QUAD1: IS A QUADRATURE INTEGRATOR OF THE GAUSS-
LEGENDRE TYPE

=====

USAGE: CALL QUAD1(FUNC,XLND,XUBND,RES,IAR,DUMMY)
FUNC = FUNCTION TO BE INTEGRATED. THIS FUNCTION
MUST BE OF THE FORM FUNCTION FUNC(ARG,DUMMY)
DUMMY = 1-DIM DUMMY ARRAY FOR PASSING DATA
TO FUNC. THIS ARRAY MUST BE DIMENTIONED
IN THE CALLING PROGRAM.
XLND = LOWER BOUND OF THE INTEGRAL
XUBND = UPPER BOUND OF THE INTEGRAL
RES = RESULT
IAR = NUMBER OF TERMS IN THE INTEGRATION
(MAX=16,MIN=2)

NOTE: FUNC MUST BE CALLED OUT AS EXTERNAL BY THE
CALLING PROGRAM

REFERENCE:
NUMERICAL ANALYSIS, Z.KOPAL, CHAPTER VII,
CHAPMAN HALL, LONDON, 1961

=====

ORIGINAL: C.L. KENNEDY OCT. 1978
C.L. KENNEDY
MOD#1-D.P. KENNEDY -- INTRODUCED GAUSS INTEGRATION FROM 2
TO 16 TERMS SEPT 1981

=====

SUBROUTINE QUAD1(FUNC,XLND,XUBND,RES,IAR,DUMMY)

COMMON /QUAD/ Z(8,16),U(8,16)

DIMENSION DUNNY(1)

DATA 2 / 8*0.000.
 3.57755236918962600.7*0.000.
 30.2745966924148300.7*0.000.
 30.86113631159405300.0.33998104358485600.6*0.000.
 30.90617984593866400.0.53846931010568300.6*0.000.
 30.93246951420315200.0.66120938646626500.0.23861918003319700.5*0.000.
 30.949791234275900.0.74153118559939400.0.40584515137739700.5*0.000.
 30.9608985649753600.0.79666647741362700.0.52553240991632900.
 30.18333464249565000.4*0.000.
 30.9681602395076200.0.83603110732533600.0.61337143270059000.
 30.32423342340380900.4*0.000.
 30.97390652851717200.0.86506336668089500.0.6794095682902400.
 30.4339539412924700.0.14887433898163100.3*0.000.
 30.97822865814605700.0.88706259976809500.0.73015200557404900.
 30.51909612920681200.0.26954315595214500.3*0.000.
 30.98156063424671900.0.90411725637047500.0.76990267419430500.
 30.58731795428661700.0.36783149899818000.0.12523340851146900.
 32*0.000.
 30.984183305471858800.0.91759839922297800.0.80157809073331000.
 30.64234933944034000.0.44849275103644700.0.23045831595513500.
 32*0.000.
 30.98628380869681200.0.92843488366357400.0.82720131506976500.
 30.68729290491168500.0.51524863635815400.0.31911236892789000.
 30.10805494670734400.0.000.
 30.9879925102048500.0.93727339240070600.0.84820658311042700.
 30.72441773136017000.0.57097217260853900.0.39415134707756300.
 30.20119409399743500.0.000.
 30.98940093499165000.0.94457502307323300.0.86563120338703200.
 30.75540440835500300.0.61787624440264400.0.4580167765722700.
 30.28160355077925900.0.09501250983763700/

DATA 4 / 8*0.000.

31.000.7*0.000.
 30.5555555555555500.0.8888888888888800.6*0.000.
 30.34785484513745400.0.65214515486294600.6*0.000.
 30.2362680805618900.0.47862867049936600.0.5688888888888800.
 35*0.000.0.1713249237917000.0.36076157304813900.
 30.46791393457269100.5*0.000.0.12948496616887000.
 30.2797053914892700.0.38183005050511900.0.41795918367349900.
 34*0.000.0.10122856329037600.0.22238103445337400.

```

$0.31370664587780700,0.36268378337836204,
$4*0.000,0.08127438836157400,0.18064816069485700,
$0.26861069440293500,0.31234707704000310,0.33023935500126000,
$3*0.000,0.06667134430868900,0.14945134915058100,
$0.21988636251598200,0.26928671930999600,0.29552422171475300,
$3*0.000,0.0556685671017400,0.12558036946499500,
$0.18629021092773400,0.23319376459199000,
$0.26200454451024700,0.27292508677790100,2*0.000,
$0.0471753338651200,0.10693932599531800,0.16007837854334600,
$0.20316742672306600,0.23349253653835500,0.24914704581340300,
$2*0.000,0.04048400476531600,0.0921214998372800,
$0.13887351021978700,0.17914598076194600,0.20781604753688900,
$0.22328318026289700,0.23255155333087400,0.000,
$0.03511946033175200,0.08015808715976000,0.12151857068790300,
$0.15220316715819400,0.18553839747793800,0.20519846372129600,
$0.21526385346315800,0.000,0.03075324199611700,
$0.07836604748810800,0.10715922046717200,0.13957067792615400,
$0.1626920581699400,0.18618100001556200,0.19843148532711200,
$0.205782492556100,0.02715245941175400,0.0622535239384800,
$0.09515851168249300,0.12462897125553400,0.1495959881657700,
$0.16915651939500300,0.18260341504492400,0.18945061045506800/

```

```

SUM=0.000
DO 10 I=1,8
IF(W(I,IAR).EQ.0) GOTO 10
ARG=(Z(I,IAR)*(XUBND-XLBNB)+XUBND+XLBNB)/2.000
TERM1=W(I,IAR)*FUNC(ARG,DUMMY)
ARG=(-Z(I,IAR)*(XUBND-XLBNB)+XUBND+XLBNB)/2.000
TERM2=0.000
IF(Z(I,IAR).NE.0.000) TERM2=W(I,IAR)*FUNC(ARG,DUMMY)
SUM=SUM+TERM1+TERM2
10 CONTINUE

```

```

RES=SUM*(XUBND-XLBNB)/2.000

```

```

RETURN
END

```

C C C

C C

```

10 / 17 / 1981      11 : 6 : 9      XINT.GW
=====
FUNCTION XINT(ARG,DUMMY)
=====
      FUNCTION XINT:REPRESENTS THE DISTRIBUTION FUNCTION FOR
      OCCUPIED ENERGY STATES IN A METAL THAT
      RESIDE ABOVE THE CONDUCTION BAND EDGE.
      THIS DISTRIBUTION IS BASED UPON THE FERMI
      -DIRAC DISTRIBUTION
=====
      DIMENSION DUMMY(10)
      EF=DUMMY(2)

      A=DSQRT(ARG)
      B=ARG-EF
      IF(B.GT.1.6D2) B=1.6D2
      IF(B.LT.-1.6D2) B=-1.6D2
      DENOM=1.0D0+EXP(B)
      XINT=A/DENOM
=====
      RETURN
      END
=====

```

APPENDIX 1-F

Program for Calculating the Saturation Current Components J_1 and J_2 ,
and the Saturation Current Using Conventional Concepts, J_c

<u>Title</u>	<u>Page</u>
MAIN	172
ROOT	178
ZERO	182
XFERMI	184
QUADI	186
DIST.	189
XINT	190
YINT	191
EFERMI	192

10 / 17 / 1991 11 : 9 : 37 CURNT.GV

=====

MAIN PROGRAM FOR CALCULATING THE ELECTRIC CURRENT IN A
P-TYPE SHOTTKY BARRIER

=====

USEAGE: REQUIRES THE SUBROUTINES

SUBROUTINE ROOT
FUNCTION ZERO
SUBROUTINE XFERMI
FUNCTION EFERMI
SUBROUTINE QUADI
FUNCTION DIST
FUNCTION XINT
FUNCTION YINT

TEMP=START OF 1/T TEMP. STEPPING
TDLT=TEMP STEP SIZE
JMAX=NUMBER OF TEMP STEPS
WC=BARRIER HEIGHT FROM TRADITIONAL THEORY
WCFLT=STEP SIZE FOR WC
IMAX=MAX. NUMBER OF STEPS FOR RATIO
EMASS=ELECTRON MASS RATIO (M*/M) FOR METAL
SEMASS=ELECTRON MASS RATIO (M*/M) FOR SEMI.
FELECT=FREE ELECTRON DENSITY IN METAL
VELECT=VALENCE ELECTRON DENSITY IN SEMI.

LUOUT=CHANNEL FOR OUTPUT

=====

ORIGINAL: D.P. KENNEDY,GAINESVILLE FLA.

=====

=====

DIMENSION DUMMY(10),A(50),B(50),C(50),D(50),E(50)
EXTERNAL ZERO,YINT,DIST

=====

ۛ ۛ ۛ

000 000 0 000 0 000

```

C
C
C
SEF0=SEF0/(8.670-5*T)
-----CALC DENSITY OF UNOCCUPIED STATES IN VALENCE BAND-----
IEXIT=0
SUM=0.000
XX=SEF0+EF*(1.000-RATIO)
XUBND=1.000-1.002/XX
IF(XUBND.LT.0.000) XUBND=0.000
EC=SEF0
25 CONTINUE
IF(IEXIT.EQ.1) GOTO 27
XLBND=XUBND
XUBND=XUBND+1.001/XX
IF(XUBND.GT.EC/XX) IEXIT=1
IF(IEXIT.EQ.1) XUBND=EC/XX
DUMMY(1)=XX
CALL QUAD1(DIST,XLBND,XUBND,RES,16,DUMMY)
SUM=SUM+RES
IF(SUM.LT.1.00-60) SUM=1.00-60
GOTO 25
C
27 CONTINUE
YY=3.000/2.000
XNV=DLOG(3.000/2.000)+DLOG(VELECT)-YY*DLOG(SEF0/XX)
XNV=XNV+BLOG(SUM)
IF(XNV.LT.-1.602) XNV=-1.602
XNV=DEXP(XNV)
P=SEF0*BOLTZ*T
WRITE(10,1122) P,XNV
1122 FORMAT(1X, SEF0=,1PD11.4,3X,XNV=,1PD11.4)
C
C
C
C
-----CALC.ET-----
ET=0.000
IF(RATIO.LT.0.000) GOTO 5
C
DUMMY(1)=FELECT
DUMMY(3)=EF
DUMMY(6)=XNV
DUMMY(7)=T
C

```

```

ARG=EF*RATIO
XX=ZERO(ARG,DUMMY)
IF (XX.GE.0.000) ET=ARG
IF (XX.LE.0.000) GOTO 5

ARG=1.00-25
XX=ZERO(ARG,DUMMY)
IF (XX.GE.0.000) ET=ARG
IF (XX.LE.0.000) GOTO 5

ET=0.000
ETMAX=1.002*EF
DLTE=EF/1.002
EPS=1.00-4

CALL FOOT(ZERO,ET,ETMAX,DLTE,EPS,0,IER,DUMMY)
IF (IER.NE.1) WRITE(LUOUT)'ROOT FOR ET NOT FOUND'
IF (IER.NE.1) STOP

5 CONTINUE

-----CALC. CURRENT ABOVE ET-----

XX=ET-EF*RATIO
XJ1=DLOG(Q)+DLOG(XNV)+DLOG(DSORT(1.000/SEMASS))
XJ1=XJ1+DLOG(DSORT(BOLTZ*T/(XMASS*2.000*PI)))-XX
IF (XJ1.LT.-1.602) XJ1=-1.602
XJ1=DEXP(XJ1)

-----CALC. CURRENT BELOW ET-----

SUM=0.000

DUMMY(2)=EF
IEXIT=0
XUBND=0.000
XX=1.000-1.502/EF
IF (XX.GT.0.000) XUBND=XX

10 CONTINUE
IF (IEXIT.EQ.1) GOTO 20
XUBND=XUBND
XUBND=XUBND+1.000

```

[illegible]

WRITE (UNIT)

NO=NO-MOULT

40 CONTINUE

END

C C

10 / 17 / 1991

11 : 12 : 59

ROUT.GV

```

=====
SUBROUTINE ROOT : LOCATES THE ROOT OF AN ARBITRARY FUNCTION
=====
USAGE : CALL ROOT (B,X,XMAX,DELX,EPS,IAR,IER,DUMMY)
WHERE : B(X,DUMMY) = ARBITRARY FUNCTION
.
. DUMMY = A 10 ELEMENT ARRAY USED FOR PASSING
. PARAMETERS TO THE FUNCTION "B"
.
. X = MIN (MAX) VALUE OF X BEGINING SEARCH
.
. XMAX = MAX (MIN) VALUE OF X DURING SEARCH
.
. DELX = INITIAL STEP SIZE
. ( +DELX INCREASES X , -DELX DECREASES X )
.
. EPS = PERMITTED FRACTIONAL ERROR
.
. IAR = ITERATION METHOD
. ( IAR = 0 BINARY CHOP )
. ( IAR = 1 METHOD OF SECANTS )
.
. IER = ERROR FLAG
. ( IER = 1 ROOT FOUND )
. ( IER = 0 ROOT NOT FOUND )
.
COMMENT : THE ROOT IS RETURNED THROUGH X . ALSO THE CALLING
. PROGRAM MUST CLASSIFY THE FUNCTION NAME
. TO BE PASSED THROUGH "B" AS EXTERNAL.
=====
ORIGINAL : APPLIED ELECTRONIC RESEARCH, GAINESVILLE, FLA. DEC. 1977
=====
MOD#1 : AERC C.L. KENNEDY NOV. 1978
. IF X REACHES XMAX SET X=0 AND RETURN
.

```



```

IF(A.LT.0.000) GOTO 15
Y=Z
GOTO 10

```

```

-----
BINARY CHOP OR METHOD OF SECANTS ?
-----

```

```

15 DEL=DELX
IF(IAR.EQ.1) GOTO 60

```

```

-----
BINARY CHOP
-----

```

```

20 Y=Z
P(1)=P(2)
30 DEL=DEL/2.000
X=X-DEL
P(2)=X
Z=B(X,DUMMY)
AB=(P(1)-P(2))/P(2)
IF(DABS(AB).LE.EPS) RETURN
A=Y#Z
P(1)=P(2)
IF (A.LT.0.000) GOTO 40
GOTO 30

```

```

C
40 Y=Z
P(1)=P(2)
50 DEL=DEL/2.000
X=X+DEL
P(2)=X
Z=B(X,DUMMY)
AB=(P(1)-P(2))/P(2)
IF(DABS(AB).LE.EPS) RETURN
A=Y#Z
P(1)=P(2)
IF (A.LT.0.000) GOTO 20
GOTO 50

```

METHOD OF SECANTS

C
C
C

```

60 Q(2)=Z
P(2)=X
P(1)=X-DEL
PREP=P(1)
Q(1)=B(DUMMY,PREP)
70 XX=(P(2)*Q(1)-P(1)*Q(2))/(Q(1)-Q(2))
YY=B(XX,DUMMY)
P(1)=P(2)
Q(1)=Q(2)
P(2)=XX
Q(2)=YY
ERROR=2ABS((P(1)-P(2))/P(2))
IF(ERROR.LE.EPS) GOTO 80
GOTO 70
80 X=XX
RETURN

```

C
C
C
C
C

ERROR RETURN X=0 IER=0

```

90 X=0.0D0
IER=0
RETURN
END

```

10 / 17 / 1981 11 : 15 : 46 ZERO.GV

```

=====
FUNCTION ZERO: CALCULATES WITHIN AN ENERGY RANGE E AND
              (E+DE) THE DIFFERENCE BETWEEN UNOCCUPIED
              STATES IN THE METAL AND ELECTRONS WITH
              A MAXWELLIAN DISTRIBUTION THAT ARE
              AVAILABLE TO OCCUPY THESE STATES
=====
ORIGINAL: D.P. KENNEDY & ASSOC. GAINESVILLE, FLA.
=====
FUNCTION ZERO(ARG,DUMMY)
  DIMENSION DUMMY(10)
  FELECT=DUMMY(1)
  EF=DUMMY(3)
  XNV=DUMMY(6)
  T=DUMMY(7)
  BOLTZ=8.6166D0
  PI=3.14159265
  XX=ARG
  IF(ODABS(XX).LE.1.0D-70) XX=1.0D-70
  TERM1=DLOG(3.0D0)+DLOG(FELECT)-3.0D0+DLOG(EF0)/2.0D0+DLOG(XX)
  XX=EF-ARG
  IF(XX.GT.1.5D2) TERM1=TERM1-XX
  IF(XX.GT.1.5D2) GOTO 10
  IF(XX.LT.-1.5D2) GOTO 10
  TERM1=TERM1-DLOG(1.0D0+DEXP(XX))
10 CONTINUE
  TERM2=-DLOG(DSORT(1.0D0/(2.0D0+PI*BOLTZ*T)))+DLOG(XNV)
  XX=ARG-RATIO*EF
  TERM2=TERM2-XX
  ZERO=TERM1-TERM2
=====

```

U

10 / 17 / 1981 11 : 16 : 38 XFERMI.GV

COMPILER DOUBLE PRECISION

SUBROUTINE XFERMI IS USED TO CALCULATE THE FERMI LEVEL
IN A METAL AT A SPECIFIED TEMP

USAGE: REQUIRES THE FOLLOWING
FUNCTION EF0
SUBROUTINE ROOT
FUNCTION XINT

ORIGINAL: D.P. KENNEDY & ASSOC.. GAINESVILLE FLA.

SUBROUTINE XFERMI (ELECT,EF0,T,EMASS,EF,LUDOUT)

DIMENSION DUMMY(10),A(50),B(50)
EXTERNAL EF0

-----CALCULATE FERMI LEVEL AT ZERO K-----

EF0=3.00*ELECT*1.0D-21/(EMASS*(3.00D/2.00D)*1.2368D1)
EF0=EF0*(2.00D/3.00D)
EF0=EF0/(8.617D-5*T)

-----CALCULATE FERMI LEVEL-----

DUMMY(1)=EF0
EF=EF0*0.75D0
EFMAX=1.0D2*EF0
DELTE=EF0*5.0D-1
EPS=1.0D-4

CALL ROOT (EFERMI,EF,EFMAX,DELTE,EPS,1,IER,DUMMY)
IF IER.NE.1) WRITE(LUOUT) ROOT NOT FOUND
IF IER.NE.1) STOP
END

10 / 17 / 1981 11 : 17 : 27 QUAD1.GV

=====

SUBROUTINE QUAD1: IS A QUADRATURE INTEGRATOR OF THE GAUSS-
LEGENDRE TYPE

=====

USAGE: CALL QUAD1(FUNC,XLND,XUBND,RES,IAR,DUMMY)
FUNC = FUNCTION TO BE INTEGRATED. THIS FUNCTION
MUST BE OF THE FORM FUNCTION FUNC(ARG,DUMMY)
DUMMY = 1-DIM DUMMY ARRAY FOR PASSING DATA
TO FUNC. THIS ARRAY MUST BE DIMENTIONED
IN THE CALLING PROGRAM.
XLND = LOWER BOUND OF THE INTEGRAL
XUBND = UPPER BOUND OF THE INTEGRAL
RES = RESULT
IAR = NUMBER OF TERMS IN THE INTEGRATION
(MAX=16,MIN=2)

NOTE:

FUNC MUST BE CALLED OUT AS EXTERNAL BY THE
CALLING PROGRAM

REFERENCE:

NUMERICAL ANALYSIS, Z.KOPAL, CHAPTER VII,
CHAPMAN HALL, LONDON, 1961

=====

ORIGIONAL:C.L. KENNEDY OCT. 1978

C.L. KENNEDY

MOD#1-D.P. KENNEDY --INTRODUCED GAUSS INTEGRATION FROM 2
TO 16 TERMS SEPT 1981

=====

SUBROUTINE QUAD1(FUNC,XLND,XUBND,RES,IAR,DUMMY)

COMMON /QUAD/ Z(8,16),W(8,16)

DIMENSION DUMMIES

DATA Z / 8*0.000,
 2.57735226918962600,7*0.000,
 \$0.7745966924140100,7*0.000,
 \$0.86113631159405300,0.33998104358485600,6*0.000,
 \$0.90617984593866400,0.53846931010568300,6*0.000,
 \$0.93246951420315200,0.66120938646626500,0.23861918608319700,5*0.000,
 \$0.94910791234275900,0.7415311859939400,0.40584515137739700,5*0.000,
 \$0.96059985649753600,0.79666847741362700,0.52553240991632900,
 \$0.18343464249565000,4*0.000,
 \$0.96816023950762600,0.83603110732663600,0.61337143270059000,
 \$0.32455142349308900,4*0.000,
 \$0.97398652881717200,0.8650633668898500,0.67940956329902400,
 \$0.43339539412924700,0.14887433898163100,3*0.000,
 \$0.97822865814605700,0.88706259976809500,0.73015200557404900,
 \$0.51909612920681200,0.26954315595234500,3*0.000,
 \$0.98150063424671900,0.90411725637047500,0.76990267419430500,
 \$0.58731795428661700,0.36783149899818000,0.12523340851146900,
 \$2*0.000,
 \$0.98418305471858800,0.91759839922297800,0.8015780907331000,
 \$0.64234933944034000,0.44849275103644700,0.23045831595513500,
 \$2*0.000,
 \$0.9862838089681200,0.9284348836357400,0.82720131506976500,
 \$0.68729290481168500,0.51524863635815400,0.31911236892789000,
 \$0.10805494870734400,0.000,
 \$0.98799251802048000,0.93727339240070600,0.84820658341042700,
 \$0.72441773136017000,0.57097217260853900,0.39415134707756300,
 \$0.20119409399743500,0.000,
 \$0.98940093499165000,0.9445502307323300,0.86563120238783200,
 \$0.7554044083500300,0.61787624440264400,0.4580167765722700,
 \$0.28160355077925900,0.09501250983763700/

DATA W / 8*0.000,
 \$1.000,7*0.000,
 \$0.55555555555555500,0.8888888888888900,6*0.000,
 \$0.34785484513745400,0.65214515486254600,6*0.000,
 \$0.236268805618900,0.47862867049936600,0.5683888888888900,
 \$5*0.000,0.1713244923917000,0.36076157304813900,
 \$0.46791393457269100,5*0.000,0.12948496616887000,
 \$0.27970539148927700,0.381830050511900,0.41795918367346900,
 \$4*0.000,0.10122856329037600,0.22238103445337400,

```

SUM=0.000
DO 10 I=1,8
  IF (W(I,IAR).EQ.0) GO TO 10
  ARG=Z(I,IAR)*XUBND-XLBN0)+XUBND+XLBN0)/2.000
  TERM=U(I,IAR)+FUNC(ARG,DUMMY)
  ARG=(-Z(I,IAR)+(XUBND-XLBN0)+XUBND+XLBN0)/2.000
  TERM2=0.000
  IF (Z(I,IAR).NE.0.000) TERM2=U(I,IAR)*FUNC(ARG,DUMMY)
  SUM=SUM+TERM1+TERM2
10 CONTINUE

RES=SUM*(XUBND-XLBN0)/2.000

RETURN
END

```

12 / 12 / 1981 11 : 22 : 35 DIST.6V

FUNCTION DIST(ARG,DUMMY)

=====

FUNCTION DIST:REPRESENTS THE DISTRIBUTION FUNCTION FOR
UNOCCUPIED ENERGY STATES IN A METAL THAT
RESIDE ABOVE THE CONDUCTION BAND EDGE.
THIS DISTRIBUTION IS BASED UPON THE FERMI
-DIRAC DISTRIBUTION

=====

DIMENSION DUMMY(10)
EFC=DUMMY(1)

A=DSORT(ARG)
B=EFC*(1.000-ARG)
IF (B.GT.1.602) B=1.602
IF (B.LT.-1.602) B=-1.602
DENOM=1.000+DEXP(B)
DIST=A/DENOM

RETURN
END

```

10 17 1981      11 12:5      XINT.00
      FUNCTION XINT(ARG,DUMMY)
      =====
      FUNCTION XINT: REPRESENTS THE DISTRIBUTION FUNCTION FOR
      OCCUPIED ENERGY STATES IN A METAL THAT
      RESIDE ABOVE THE CONDUCTION BAND EDGE.
      THIS DISTRIBUTION IS BASED UPON THE FERMI
      -DIRAC DISTRIBUTION
      =====
      DIMENSION DUMMY(:)
      EF=DUMMY(2)
      A=DSQRT(ARG)
      B=ARG-EF
      IF(B.GT.1.6D2) B=1.6D2
      IF(B.LT.-1.6D2) B=-1.6D2
      DENOM=1.0D2+DEXP(B)
      XINT=A/DENOM
      RETURN
      END

```

```

10 / 17 / 1981      11 : 21 : 34      YINT.00
=====
FUNCTION YINT(ARG,DUMMY)
=====
      FUNCTION YINT IS THE INTEGRAND FOR CALCULATING THE
      ELECTRIC CURRENT IN A P-TYPE SCHOTTKY
      BARRIER IN THE REGION BELOW ET
=====
      ORIGINAL: D.P. KENNEDY & ASSOC. GAINESVILLE FLA.
=====
      DIMENSION DUMMY(10)
      EF=DUMMY(2)
=====
      IF(ARG.GT.1.6D2) ARG=1.6D2
      IF(ARG.LT.-1.6D2) ARG=-1.6D2
      A=DLOG(ARG)
      B=EF-ARG
      IF(B.GT.1.6D2) B=1.6D2
      IF(B.LT.-1.6D2) B=-1.6D2
      DENOM=1.0D0+DEXP(B)
      IF(DENOM.GT.1.0D70) DENOM=1.0D70
      IF(DENOM.LT.-1.0D70) DENOM=-1.0D70
      DENOM=DLOG(DENOM)
      YINT=A-B
      IF(YINT.GT.1.6D2) YINT=1.6D2
      IF(YINT.LT.-1.6D2) YINT=-1.6D2
      YINT=DEXP(YINT)
=====
      RETURN
      END
=====

```

EFERMI.SV

11 : 22 : 12

10 / 17 / 1981

```

=====
FUNCTION EFERMI: IS USED TO CALC. THE FERMI LEVEL IN A
METALLIC CONDUCTOR

USAGE:  REQUIRES SUBROUTINE QUAD1 AND FUNCTION XINT
=====

ORIGINAL: D.P. KENNEDY, GAINESVILLE FLA.
=====

FUNCTION EFERMI(EF, DUMMY)
  DIMENSION DUMMY(10)
  EXTERNAL XINT
  -----INTEGRATE FROM 0 TO INF-----

  EF0=DUMMY(1)
  DUMMY(2)=EF
  SUM=0.000
  XX=EF-1.20
  IF(XX.GT.0.200) SUM=2.000*(XX*(3.000/3.000)/3.000
  XUBND=0.000
  IF(XX.GT.0.200) XUBND=XX
  10 CONTINUE
  XLBND=XUBND
  XUBND=XUBND+1.001
  XX=XUBND-EF
  IF(XX.GT.1.002) GOTO 30
  CALL QUAD1(XINT, XLBND, XUBND, RES, 16, DUMMY)
  SUM=SUM+RES
  GOTO 10

30 CONTINUE
  EFERMI=1.000-3.000*EF0+(-3.000/2.000)*SUM/2.000

```

1-2 1-4 1-6 1-8

APPENDIX 1-G

Program for Calculating the Volt-Ampere Characteristics of a Schottky Barrier Based Upon the Concepts Developed During This Research, and Upon Traditional Concepts of Device Operation

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EQU	205
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XFERMI.	212
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DIST.	217
XINT.....	218
YINT	219
EFERMI	220

[illegible]

MAIN PROGRAM FOR CALCULATION OF CURRENT/VOLTAGE CURVES FOR A P-TYPE SCHOTTKY BARRIER

```

      USAGE:  REQUIRES THE SUBROUTINES
              SUBROUTINE ROOT
              FUNCTION ZERO
              SUBROUTINE XFERRI
              SUBROUTINE QUAD1
              SUBROUTINE XTERRR
              FUNCTION DIST
              FUNCTION XINT
              FUNCTION YINT
              FUNCTION EQU

```

```

ACCEPTR=ACCEPTOR DENSITY IN SILICON
TEMP=TEMPERATURE OF DEVICE OPERATION
BARRIER=BARRIER HEIGHT FROM TRADITIONAL THEORY
WCDLT=STEP SIZE FOR BARRIER HEIGHT
INAX=NUMBER OF STEPS FOR WC
EMASS=ELECTRON MASS RATIO (M*/M) FOR METAL
SCMASS=ELECTRON MASS RATIO (M*/M) FOR SEMI.
FELECT=FREE ELECTRON DENSITY IN METAL
DLTNC=STEP SIZE FOR FELECT
LMAX=NUMBER OF FELECT STEPS
VFELECT=VALENCE ELECTRON DENSITY IN SEMI.
WAPPL=START OF APPLIED VOLTAGE STEPPING
WCDLT=SIZE OF STEP FOR VAPPL
JMAX=NUMBER OF VAPPL STEPS

```

LUOUT=CHANNEL FOR OUTPUT

ORIGINAL: D.P. KENNEDY, GAINESVILLE FLA.


```

IF(XUBND.GT.EC/XX) IEXI=1
IF(IEXI.EQ.1) XUBND=EC/XX
DUMMY(1)=XX
CALL QUAD1(DIST,XLBRD,XUBND,RES,16,DUMMY)
SUM=SUM+RES
IF(SUM.LT.1.0D-60) SUM=1.0D-60
GOTO 25

C 27 CONTINUE
YY=3.0D0/2.0D0
XNV=DLOG(3.0D0/2.0D0)+DLOG(VELECT)-YY*DLOG(SEF0/XX)
XNV=XNV+DLOG(SUM)
IF(XNV.LT.-1.6D2) XNV=-1.6D2
XNV=DEXP(XNV)
-----CALC.ET-----
ET=0.0D0
IF(RATIO.LT.0.0D0) GOTO 5

DUMMY(1)=XNC
DUMMY(3)=EF
DUMMY(6)=XNV
DUMMY(7)=T

C ARG=EF*RATIO
XX=ZERO(ARG,DUMMY)
IF(XX.GE.0.0D0) ET=ARG
IF(XX.GE.0.0D0) GOTO 5

C ARG=1.0D-25
XX=ZERO(ARG,DUMMY)
IF(XX.GE.0.0D0) ET=ARG
IF(XX.GE.0.0D0) GOTO 5

C ET=0.0D0
ETMAX=1.0D2*EF
DLTE=EF/1.0D2
EPS=1.0D-4

C CALL ROOT(ZERO,ET,ETMAX,DLTE,EPS,0,IER,DUMMY)
IF(IER.NE.1) WRITE(LUOUT) 'ROOT FOR ET NOT FOUND'

```

```

IF(IER.NE.1) STOP
5 CONTINUE
-----CALC. CURRENT ABOVE ET-----
XX=ET-EF*RATIO
XJ1=DLOG(Q)+DLOG(XNV)+DLOG(DSQRT(1.0D0/SEMASS))
XJ1=XJ1+DLOG(DSQRT(BOLTZ*T/(XMASS*2.0D0*PI)))-XX
IF(XJ1.LT.-1.6D2) XJ1=-1.6D2
XJ1=DEXP(XJ1)
-----CALC. CURRENT BELOW ET-----
SUM=0.0D0
DUMMY(2)=EF
IEXIT=0
XUBND=0.0D0
XX=1.0D0-1.5D2/EF
IF(XX.GT.0.0D0) XUBND=XX
10 CONTINUE
IF(IEXIT.EQ.1) GOTO 20
XLBND=XUBND
XUBND=XUBND+1.0D0
IF(XUBND.GE.ET) IEXIT=1
IF(IEXIT.EQ.1) XUBND=ET
DUMMY(1)=EF
IF(XUBND-XLBND.LT.1.0D-50) GOTO 15
CALL QUAD1(YINT,XLBND,XUBND,RES,16,DUMMY)
SUM=SUM+RES
15 CONTINUE
GOTO 10
IF(SUM.LT.1.0D-60) SUM=1.6D-60
20 CONTINUE
XJ2=DLOG(3.0D0)+DLOG(XNC)-3.0D0*DLOG(EF0)/2.0D0+DLOG(DSQRT(XMASS))
XJ2=XJ2+DLOG(SUM)+DLOG(DSQRT(1.0D0/EMASS))+DLOG(Q)
IF(XJ2.LT.-1.6D2) XJ2=-1.6D2
XJ2=DEXP(XJ2)

```

```
C
C
-----CALC. CURRENT USING CONVENTIONAL THEORY-----
XJC=DLOG(Q)+DLOG(XVU)+DLOG(DSORT(1.0D0/SEMASS))
XJC=XJC+DLOG(DSQRT(BOLTZ*T/(2.0D0*PI*XMASS)))-EF*(1.0D0-RATIO)
IF(XJC.LT.-1.6D2) XJC=-1.6D2
XJC=DEXP(XJC)

C
C
----PRINT RESULTS-----
XJT=XJ1+XJ2
XJT=DLOG(XJT)
XX=XV/(BOLTZ*T)
IF(XX.GT.1.6D2) XX=1.6D2
XX=1.0D0-DEXP(-XX)
IF(XX.LT.1.0D-7D) XX=1.0D-7D
XX=DLOG(XX)
XJT=XJT+XX
IF(XJT.GT.1.6D2) XJT=1.6D2
IF(XJT.LT.-1.6D2) XJT=-1.6D2
XJT=DEXP(XJT)

C
XJC=DLOG(XJC)
XJC=XJC+XX
IF(XJC.GT.1.6D2) XJC=1.6D2
IF(XJC.LT.-1.6D2) XJC=-1.6D2
XJC=DEXP(XJC)

C
EB=EF*RATIO*BOLTZ*T
EF=EF*BOLTZ*T
EF=EF*BOLTZ*T
ET=ET*BOLTZ*T

C
WRITE(LUOUT,1000) EF,EB,XV,ET
WRITE(LUOUT,1010) XJ1,XJ2,XJC,XJT
1000 FORMAT('X','EF=',1PD12.5,3X,'EB=',1PD12.5,3X,'VAPPL=',1PD12.5,
      &3X,'ET=',1PD12.5)
1010 FORMAT('XJ','XJ1=',1PD12.5,3X,'XJ2=',1PD12.5,3X,'XJC=',1PD12.5
      &,3X,'XJT=',1PD12.5,/)

C
XV=XV+VDLT
30 CONTINUE
WC=WC+WCDLT
```

40 CONTINUE
XNC=XNC+DLINC
50 CONTINUE
END

10 / 17 / 1981

11 : 39 : 46

XTEMPR,6V

SUBROUTINE XTEMPR: IS USED TO CALCULATE MANY TEMP DEPENDENT
PROPERTIES OF SILICON, IN ADDITION TO THE
DIFF POTENTIAL OF A PT-SI BARRIER

XION=IONIZED BORON ATOMS (CM**3)
ENSUBI=NI (CM**3)
VDIFF=DIFF POTENTIAL (VOLTS)
EIF=EI-EF IN EV
EIV=EI-EV IN EV
TEMP=TEMPERATURE DEG.K
HOLES=HOLE DENSITY (CM**3)
EGAP=ENERGY GAP IN EV
ACCPTR=ACCPTR DENSITY (CM**3)
BARRER=ENERGY BARRIER (EV) FOR VDIFF CALC
BOLTZ=BOLTZMANN CONSTANT AT 300 DEG. K

LUOUT=OUTPUT CHANNEL

USAGE: REQUIRES SUBROUTINE ROOT AND FUNCTION EQU

ORIGINAL: D.P. KENNEDY & ASSOC., GAINESVILLE FLA.

SUBROUTINE XTEMPR(XION,ENSUBI,VDIFF,EIF,EIV,TEMP,HOLES,EGAP,BOLTZ,
&ACCPTR,BARRIER,LUOUT)
DIMENSION DUMMY (11)
EXTERNAL EQU

T=TEMP/3.D2

EGAP=1.165-7.242E-3*T-3.664E-2*T*T

EIV=EGAP/2.D0-1.306E-2*T

ENSUBI=3.925D19*T*DSORT(T)*DEXP(-EGAP/(2.D0*BOLTZ*T))

AD-A113 211 KENNEDY (D P) AND ASSOCIATES INC GAINESVILLE FL F/0 20/12
INVESTIGATION OF THE CURRENT VOLTAGE RELATIONSHIP FOR LOW BARRIER-ETC(U)
FEB 82 D P KENNEDY F19628-80-C-0020

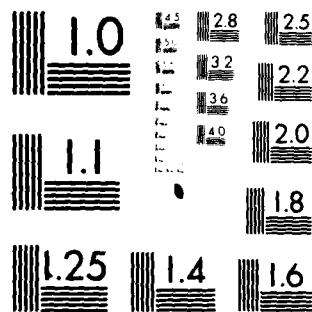
KENNEDY (D P) AND ASSOCIATES INC GAINESVILLE FL F/O 20/12
INVESTIGATION OF THE CURRENT VOLTAGE RELATIONSHIP FOR LOW BARRI--ETC(U)
FEB 82 D P KENNEDY F19628-80-C-0020

RADC-TR-82-13

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END
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MICROCOPY RESOLUTION TEST CHART
NATIONAL BUREAU OF STANDARDS-1963-A

C C

```
DUMMY(1)=EGAP
DUMMY(2)=EIV
DUMMY(3)=ENSUBI
DUMMY(4)=T
DUMMY(5)=BOLTZ
DUMMY(6)=BRRIER
DUMMY(7)=ACCPTR
```

C

```
EIF=EIV
EIFMX=-EIV
DLTEI=-EIV/2.0D1
```

C

```
CALL ROOT(EQU,EIF,EIFMX,DLTEI,1.0D-6,0,IER,DUMMY)
```

C

```
IF (IER.NE.1) WRITE(LUOUT)'ROOT NOT FOUND IN XTEMP'
```

C

```
XION=DUMMY(8)
EAF=DUMMY(9)
EFV=DUMMY(10)
HOLES=DUMMY(11)
```

C

```
VDIFF=BRRIER-EFV
```

C

```
RETURN
END
```

```

10 / 17 / 1981      11 : 41 : 1      EQU.GV

C      FUNCTION EQU(EIF,DUMMY)
C      DIMENSION DUMMY(11)
      EGAP=DUMMY(1)
      EIF=DUMMY(2)
      ENSUBI=DUMMY(3)
      T=DUMMY(4)
      BOLTZ=DUMMY(5)
      BRRIER=DUMMY(6)
      ACCPTR=DUMMY(7)
C
      EFV=EIF-EIF
      EAF=4.38D-2-3.037D-8*ACCPTR*(1.0/3.0)-EFV
      XION=1.0D0/(1.0+(4.0+2.0/DEXP(4.4D-2/(BOLTZ*T)))*DEXP(EAF/(BOLTZ*T)))
      XION=XION*ACCPTR
C
      HOLES=ENSUBI*DEXP(EIF/(BOLTZ*T))
      EQU=(HOLES-XION)/ACCPTR
C
      DUMMY(8)=XION
      DUMMY(9)=EAF
      DUMMY(10)=EFV
      DUMMY(11)=HOLES
C
      RETURN
      END

```

10 / 17 / 1981

11 : 41 : 27

ROOT.6V

SUBROUTINE ROOT : LOCATES THE ROOT OF AN ARBITRARY FUNCTION

USAGE : CALL ROOT (B,X,XMAX,DELX,EPS,IAR,IER,DUMMY)

WHERE : B(X,DUMMY) = ARBITRARY FUNCTION

DUMMY = A 10 ELEMENT ARRAY USED FOR PASSING
PARAMETERS TO THE FUNCTION "B"

X = INITIAL VALUE OF X BEGINNING SEARCH

XMAX = MAX (MIN) VALUE OF X DURING SEARCH

DELX = INITIAL STEP SIZE
(+DELX INCREASES X , -DELX DECREASES X)

EPS = PERMITTED FRACTIONAL ERROR

IAR = ITERATION METHOD
(IAR = 0 BINARY CHOP)
(IAR = 1 METHOD OF SECANTS)

IER = ERROR FLAG
(IER = 1 ROOT FOUND)
(IER = 0 ROOT NOT FOUND)

COMMENT : THE ROOT IS RETURNED THROUGH X . ALSO THE CALLING
PROGRAM MUST CLASSIFY THE FUNCTION NAME
TO BE PASSED THROUGH "B" AS EXTERNAL.

ORIGINAL : APPLIED ELECTRONIC RESEARCH, GAINESVILLE, FLA. DEC. 1977

MODN1 : AERC C.L. KENNEDY NOV. 1978
IF X REACHES XMAX SET X=0 AND RETURN

```

MOD#2 : AERC D.P. KENNEDY NOV 1978
      . INTRODUCED ERROR FLAG IER
      .
MOD#3 : AERC D.P. KENNEDY NOV. 1978
      . EPS=FRACTIONAL CHANGE IN X
      . METHOD OF SECANTS INTRODUCED
      .
MOD#4 : AERC C.L. KENNEDY DECEMBER 1978
      . ALL DUMMY VARIABLES PASSED
      . THROUGH ARRAY DUMMY
=====

```

```

SUBROUTINE ROOT (B,X,XMAX,DELX,EPS,IAR,IER,DUMMY)

```

```

      * IMPLICIT REAL*8(A-H,O-Z)

```

```

      DIMENSION P(2),Q(2),DUMMY(1)

```

```

      IF (DELX.EQ.0.0D0) GOTO 90
      IER=1

```

```

      P(1)=0.0D0

```

```

      P(2)=0.0D0

```

```

      Q(1)=0.0D0

```

```

      Q(2)=0.0D0

```

```

      Y=B(X,DUMMY)

```

```

      P(1)=X

```

```

-----
STEP TO BRACKET ROOT
-----

```

```

10 X=X+DELX

```

```

      P(2)=X

```

```

      IF (DELX.GT.0.0.AND.X.GE.XMAX) GOTO 90

```

```

      IF (DELX.LT.0.0.AND.X.LE.XMAX) GOTO 90

```

```

      Z=B(X,DUMMY)

```

```

      AB=(P(1)-P(2))/P(2)

```

```

      IF (DABS(AB).LE.EPS) RETURN

```

```

      A=Y*Z

```

```

      P(1)=P(2)

```

```

IF(A.LT.0.000) GOTO 15
Y=Z
GOTO 10

```

C
C
C
C
C
C

B I N A R Y C H O P O R M E T H O D O F S E C A N T S ?

```

15 DEL=DELX
IF(IAR.EQ.1) GOTO 60

```

C
C
C
C
C
C

B I N A R Y C H O P

```

20 Y=Z
P(1)=P(2)
30 DEL=DEL/2.000
X=X-DEL
P(2)=X
Z=B(X,DUMMY)
AB=(P(1)-P(2))/P(2)
IF(DABS(AB).LE.EPS) RETURN
A=Y+Z
P(1)=P(2)
IF (A.LT.0.000) GOTO 40
GOTO 30

```

C

```

40 Y=Z
P(1)=P(2)
50 DEL=DEL/2.000
X=X+DEL
P(2)=X
Z=B(X,DUMMY)
AB=(P(1)-P(2))/P(2)
IF(DABS(AB).LE.EPS) RETURN
A=Y+Z
P(1)=P(2)
IF (A.LT.0.000) GOTO 20
GOTO 50

```

C
C

METHOD OF SECANTS

```

60 Q(2)=Z
P(2)=X
P(1)=Y-DEL
PREP=P(1)
Q(1)=B DUMMY,PREP)
70 XX=(P(2)*Q(1)-P(1)*Q(2))/(Q(1)-Q(2))
YY=B(XX,DUMMY)
P(1)=P(2)
Q(1)=Q(2)
P(2)=XX
Q(2)=YY
ERROR=DABS((P(1)-P(2))/P(2))
IF(ERROR.LE.EPS) GOTO 80
GOTO 70
80 X=XX
RETURN
-----
ERROR RETURN X=0 IER=0
-----
90 X=0.000
IER=0
RETURN
END

```

C C C C C

END-004

RETURN
END

0

10 / 17 / 1981 11 : 45 : 5 XFERMI.GV

COMPILER DOUBLE PRECISION

=====

SUBROUTINE XFERMI IS USED TO CALCULATE THE FERMI LEVEL
IN A METAL AT A SPECIFIED TEMP

USAGE: REQUIRES THE FOLLOWING
FUNCTION EFERMI
SUBROUTINE ROOT
FUNCTION XINT

=====

ORIGINAL: D.P. KENNEDY & ASSOC., GAINESVILLE FLA.

=====

SUBROUTINE XFERMI (ELECT,EF0,T,EMASS,EF,LUOUT)

DIMENSION DUMMY(10),A(50),B(50)
EXTERNAL EFERMI

-----CALCULATE FERMI LEVEL AT ZERO K-----

EF0=3.00*ELECT*1.0D-21/(EMASS*(3.00D/2.00D)*1.2368D1)
EF0=EF0*(2.00D/3.00D)
EF0=EF0/(8.617D-5*T)

-----CALCULATE FERMI LEVEL-----

DUMMY(1)=EF0
EF=EF0*0.75D0
EFMAX=1.0D2*EF0
DELTE=EF0*5.0D-1
EPS=1.0D-4

ALW014800

```
CALL ROOT (EFERMI,EF,EFMAX,DELTE,EPS,1,IER,DUMMY)  
IF(IER.NE.1) WRITE(LUOUT)'ROOT NOT FOUND'  
IF(IER.NE.1) STOP  
END
```

10 / 17 / 1981 11 : 45 : 54 QUAD1.GV

=====

SUBROUTINE QUAD1: IS A QUADRATURE INTEGRATOR OF THE GAUSS-
 LEGENDRE TYPE

=====

USAGE: CALL QUAD1(FUNC,XLBD,XUBND,RES,IAR,DUMMY)
 FUNC =FUNCTION TO BE INTEGRATED. THIS FUNCTION
 MUST BE OF THE FORM FUNCTION FUNC(ARG,DUMMY)
 DUMMY = 1-DIM DUMMY ARRAY FOR PASSING DATA
 TO FUNC. THIS ARRAY MUST BE DIMENTIONED
 IN THE CALLING PROGRAM.
 XLBD = LOWER BOUND OF THE INTEGRAL
 XUBND = UPPER BOUND OF THE INTEGRAL
 RES = RESULT
 IAR = NUMBER OF TERMS IN THE INTEGRATION
 (MAX=16,MIN=2)

NOTE:

FUNC MUST BE CALLED OUT AS EXTERNAL BY THE
 CALLING PROGRAM

REFERENCE:

NUMERICAL ANALYSIS, Z.KOPAL, CHAPTER VII,
 CHAPMAN HALL, LONDON, 1961

=====

ORIGINAL:C.L. KENNEDY OCT. 1978
 C.L. KENNEDY
 MODN1-D.P. KENNEDY --INTRODUCED GAUSS INTEGRATION FROM 2
 TO 16 TERMS SEPT 1981

=====

SUBROUTINE QUAD1(FUNC,XLBD,XUBND,RES,IAR,DUMMY)

COMMON /QUAD/ Z(8,16),W(8,16)

DIMENSION DUMMY(1)

DATA Z / 8*0.000,
 3.57735026918962600,7*0.000,
 0.77459666924148300,7*0.000,
 0.86113631159405300,0.33998104358485600,6*0.000,
 0.90617984593866400,0.53846931010568300,6*0.000,
 0.93246951420315200,0.66120938646626500,0.23861918609319700,5*0.000,
 0.94910791234275900,0.74153118559939400,0.40584515137739700,5*0.000,
 0.96028985649753600,0.79666647741362700,0.52553240991632900,
 0.18343464249565000,4*0.000,
 0.96816023950762600,0.83603110732663600,0.61337143270059000,
 0.32425342340380900,4*0.000,
 0.97390652851717200,0.86506336668898500,0.67940956829902400,
 0.4339539412924700,0.14887433898163100,3*0.000,
 0.97822865814605700,0.88706259976809500,0.73015200557404900,
 0.51909612920681200,0.26954315595234500,3*0.000,
 0.98156063424671900,0.90411725637047500,0.76990267419430500,
 0.58731795428661700,0.36783149899818000,0.12523340051148900,
 0.98418305471858800,0.91759839922297800,0.80157809073331000,
 0.64244933944034000,0.44849275103644700,0.23045831595513500,
 0.982838089681200,0.92843488366357400,0.82720131506976500,
 0.68729290481168500,0.51524863635815400,0.31911236892789000,
 0.108054987073400,0.000,
 0.98799251802048500,0.93727339240070600,0.84820658341042700,
 0.72441773136017000,0.57097217260853900,0.39415134707756300,
 0.20119409399743500,0.000,
 0.989400093499165000,0.94457502307323300,0.86563120238783200,
 0.75540440835500300,0.61787624440264400,0.4580167765702700,
 0.28160355077925900,0.09501250983763700/

DATA W / 8*0.000,
 0.1000,7*0.000,
 0.55555555555555500,0.88888888888888900,6*0.000,
 0.34785484513745400,0.65214515486254600,6*0.000,
 0.2382688505618900,0.47862867049936600,0.56838383838383900,
 0.17132449237917000,0.36076157304813900,
 0.46791393457269100,5*0.000,0.12948496616887000,
 0.27970539148927700,0.381830050511900,0.41795918367346900,
 0.10122856329037600,0.22238103445337400,

```

$0.31370644587788700,0.36268378337836200,
$4*0.000,0.08127438836157400,0.18064816069485700,
$0.2606189640293500,0.31234707704000300,0.33023735500126000,
$3*0.000,0.0666713443086800,0.14945134915058100,
$0.2190866251598200,0.26926671930999600,0.29552422471475300,
$3*0.000,0.05566856711617400,0.12558036946490500,
$0.18629021092773400,0.23319376459199000,
$0.26280454451024700,0.27292508677790100,2*0.000,
$0.04717533638651200,0.10693932599531800,0.16007832854334600,
$0.20316742672306600,0.23349253653835500,0.24914704581340300,
$2*0.000,0.04048400476531600,0.09212149983772800,
$0.13887351021978700,0.17814598076194600,0.20781604753688900,
$0.22628318026289700,0.23255155323087400,0.000,
$0.03511946033175200,0.08015808715976000,0.12151857068790300,
$0.15720316715819400,0.1853389747793800,0.20519846372129600,
$0.21526385346315800,0.000,0.03075324199611700,
$0.07036684748010800,0.10715922046717200,0.13957067792615400,
$0.16626920581699400,0.18616100001556200,0.19843148532711200,
$0.20257824192556100,0.02715245941175400,0.06226552393864800,
$0.09515851168249300,0.12462897125553400,0.14959598881657700,
$0.16915651939500300,0.18260341504492400,0.18945061045506800/

```

```

SUM=0.000
DO 10 I=1,8
  IF(W(I,IAF).EQ.0) GOTO 10
  ARG=(Z(I,IAF)*(XUBND-XLBNB)+XUBND+XLBNB)/2.000
  TERM1=W(I,IAF)*FUNC(ARG,DUMMY)
  ARG=(-Z(I,IAF)*(XUBND-XLBNB)+XUBND+XLBNB)/2.000
  TERM2=0.000
  IF(Z(I,IAF).NE.0.000) TERM2=W(I,IAF)*FUNC(ARG,DUMMY)
  SUM=SUM+TERM1+TERM2
10 CONTINUE
RES=SUM*(XUBND-XLBNB)/2.000
RETURN
END

```

```

10 / 17 / 1981          11 : 49 : 2          DIST.60

FUNCTION DIST(ARG,DUMMY)

=====
FUNCTION DIST:REPRESENTS THE DISTRIBUTION FUNCTION FOR
      UNOCCUPIED ENERGY STATES IN A METAL THAT
      RESIDE ABOVE THE CONDUCTION BAND EDGE.
      THIS DISTRIBUTION IS BASED UPON THE FERMI
      -DIRAC DISTRIBUTION
=====

DIMENSION DUMMY(10)
EFC=DUMMY(1)

A=DSORT(ARG)
B=EFC*(1.0D0-ARG)
IF(B.GT.1.6D2) B=1.6D2
IF(B.LT.-1.6D2) B=-1.6D2
DENOM=1.0D0+DEXP(B)
DIST=A/DENOM

=====
RETURN
END
=====

```

```

10 / 17 / 1991      11 : 49 : 32      XINT.0V
FUNCTION XINT(ARG,DUMMY)
=====
FUNCTION XINT: REPRESENTS THE DISTRIBUTION FUNCTION FOR
      OCCUPIED ENERGY STATES IN A METAL THAT
      RESIDE ABOVE THE CONDUCTION BAND EDGE.
      THIS DISTRIBUTION IS BASED UPON THE FERMI
      -DIRAC DISTRIBUTION
=====
DIMENSION DUMMY(10)
EF=DUMMY(2)

A=DSORT(ARG)
B=ARG-EF
IF(B.GT.1.6D2) B=1.6D2
IF(B.LT.-1.6D2) B=-1.6D2
DENOM=1.0D0+DEXP(B)
XINT=A/DENOM

RETURN
END

```

10 / 17 / 1981 11 : 50 : 1 YINT.GV

FUNCTION YINT(ARG,DUMMY)

=====

FUNCTION YINT IS THE INTEGRAND FOR CALCULATING THE
ELECTRIC CURRENT IN A P-TYPE SCHOTTKY
BARRIER IN THE REGION BELOW ET

=====

ORIGINAL: D.P. KENNEDY & ASSOC. GAINESVILLE FLA.

=====

DIMENSION DUMMY(10)
EF=DUMMY(2)

IF(ARG.GT.1.6D2) ARG=1.6D2
IF(ARG.LT.-1.6D2) ARG=-1.6D2
A=DLOG(ARG)
B=EF-ARG
IF(B.GT.1.6D2) B=1.6D2
IF(B.LT.-1.6D2) B=-1.6D2
DENOM=(1.0D0+DEXP(B))
IF(DENOM.GT.1.0D70) DENOM=1.0D70
IF(DENOM.LT.-1.0D70) DENOM=-1.0D70
DENOM=DLOG(DENOM)
YINT=A-B
IF(YINT.GT.1.6D2) YINT=1.6D2
IF(YINT.LT.-1.6D2) YINT=-1.6D2
YINT=DEXP(YINT)

RETURN
END

10 / 17 / 1981 11 : 50 : 39 EFERMI.GV

=====

FUNCTION EFERMI: IS USED TO CALC. THE FERMI LEVEL IN A
METALLIC CONDUCTOR

USAGE: REQUIRES SUBROUTINE QUAD1 AND FUNCTION XINT

=====

ORIGINAL: D.P. KENNEDY, GAINESVILLE FLA.

=====

FUNCTION EFERMI(EF,DUMMY)
DIMENSION DUMMY(10)
EXTERNAL XINT

-----INTEGRATE FROM 0 TO INF-----

```

EF0=DUMMY(1)
DUMMY(2)=EF
SUM=0.000
XX=EF-1.201
IF(XX.GT.0.000) SUM=2.000*(XX*(3.000/2.000))/3.000
XUBND=0.000
IF(XX.GT.0.000) XUBND=XX
10 CONTINUE
XLBND=XUBND
XUBND=XUBND+1.001
XX=XUBND-EF
IF(XX.GT.1.002) GOTO 30
CALL QUAD1(XINT,XLBND,XUBND,RES,16,DUMMY)
SUM=SUM+RES
GOTO 10

```

```

30 CONTINUE
EFERMI=1.000-3.000*EF0+((-3.000/2.000)*SUM/2.000

```

RETURN
END

APPENDIX I-H

Program for Calculating Many Equilibrium Characteristics of Silicon
Throughout a Specified Range of Temperature

<u>Title</u>	<u>Page</u>
MAIN	224
XTEMPR	226
EQU	228

[illegible]

MAIN PROGRAM FOR CALCULATING THE EQUILIBRIUM CHARACTERISTICS OF P-TYPE SILICON VS. TEMPERATURE

THE CHARACTERISTICS CALCULATED ARE:

- XION=IONIZED ACCEPTOR DENSITY
- VDIFF=DIFFUSION POTENTIAL FOR A GIVEN BARRIER
- EIF=FERMI ENERGY DISTANCE FROM INTRINSIC FERMI ENERGY, EI---IN EV
- EIV=INTRINSIC FERMI ENERGY, EF, DISTANCE FROM THE VALENCE BAND EDGE, EC---IN EV
- HEQ=EQUILIBRIUM HOLE DENSITY IN SILICON
- ENSUBI= INTRINSIC HOLE/ELECTRON DENSITY AT SPECIFIED TEMP.
- EGAP=ENERGY GAP OF FORBIDDEN BAND

USAGE: REQUIRES SUBROUTINE XTEMPR AND FUNCTION EQU

```

BARRIER=ASSUMED BARRIER AT SI/METAL INTERFACE
TEMP=STARTING STEP FOR TEMPERATURE
TDLT=STEP SIZE FOR TEMP
IMAX=NUMBER OF TEMP STEPS
ACCPTR=STARTING STEP FOR ACCEPTOR DENSITY
ADLT=STEP SIZE FOR ACCPTR
JMAX=NUMBER OF ACCPTR STEPS

LUOUT=CHANNEL FOR OUTPUT

```

ORIGINAL: D.P. KENNEDY & ASSOC., GAINESVILLE, FLA.

-----INITIALIZE MISC CONSTANTS-----

```

C      ACCPTR=1.0D11
      ADLT=1.0D1
      JMAX=7
      TEMP=7.0D1
      TDLT=1.0D1
      IMAX=24
      BRRIER=0.27D0
      BOLTZ=.02585D0

C      LUOUT=10

C      -----TOP OF ACCPTR STEPPING LOOP-----
C
C      DO 50 J=1,JMAX
C      ACCPTR=ACCPTR*1.0D1
C      WRITE(LUOUT,1111) ACCPTR
C      1111 FORMAT(1X,1PD10.3)
C
C      -----TOP OF TEMP STEPPING LOOP-----
C
C      T=TEMP
C      DO 10 I=1,IMAX
C
C      CALL XTEMPR(XION,ENSUBI,VDIFF,EIV,EIV,I,HULES,EGAP,BOLTZ,ACCPTR,
C      &BRRIER,LUOUT)
C      WRITE(LUOUT,1000) T,XION,HULES,ENSUBI,EGAP,EIV,EIV,VDIFF
C      1000 FORMAT(1X,T=,F6.1,3X,XION=,1PD10.3,3X,HULES=,1PD10.3,3X,
C      &NI=,1PD10.3,3X,EG=,1PD9.2,3X,EIV=,1PD9.2,3X,EIV=,
C      &1PD9.2,3X,VDIFF=,1PD9.2)
C
C      T=T+TDLT
C      10 CONTINUE
C
C      50 CONTINUE
C      END

```

10 / 17 / 1981 11 : 59 : 4 XTEMPR.GV

=====

SUBROUTINE XTEMPR: IS USED TO CALCULATE MANY TEMP DEPENDENT
PROPERTIES OF SILICON, IN ADDITION TO THE
DIFF POTENTIAL OF A PT-SI BARRIER

XION=IONIZED BORON ATOMS (CM**-3)
ENSUBI=NI (CM**-3)
VDIFF=DIFF POTENTIAL (VOLTS)
EIF=EI-EF IN EV
EIV=EI-EV IN EV
TEMP=TEMPERATURE DEG.K
HOLES=HOLE DENSITY (CM**-3)
EGAP=ENERGY GAP IN EV
ACCPTR=ACCPTR DENSITY (CM**-3)
BARRER=ENERGY BARRIER (EV) FOR VDIFF CALC
BOLTZ=BOLTZMANN CONSTANT AT 300 DEG. K

LUDUT=OUTPUT CHANNEL

=====

USAGE: REQUIRES SUBROUTINE ROOT AND FUNCTION EQU

=====

ORIGINAL: D.P. KENNEDY & ASSOC.. GAINESVILLE FLA.

=====

SUBROUTINE XTEMPR(XION, ENSUBI, VDIFF, EIF, EIV, TEMP, HOLES, EGAP, BOLTZ,
*ACCPTR, BARRIER, LUDUT)
DIMENSION DUMMY (11)
EXTERNAL EQU

T=TEMP/3.D2
EGAP=1.165-7.242D-3*T-3.664D-2*T*T
EIV=EGAP/2.D0-1.306D-2*T
ENSUBI=3.925D19*T*DSORT(1)*DEXP(-EGAP/(2.D0*BOLTZ*T))

C C

```
DUMMY(1)=EGAP
DUMMY(2)=EIV
DUMMY(3)=ENSUBI
DUMMY(4)=T
DUMMY(5)=BOLTZ
DUMMY(6)=BRRIER
DUMMY(7)=ACCPTR
```

C

```
EIF=EIV
EIFMX=-EIV
DLTEI=-EIV/2.0D1
```

C

```
CALL ROOT(EQU,EIF,EIFMX,DLTEI,1.0D-6,0,IER,DUMMY)
```

C

```
IF (IER.NE.1) WRITE(LUOUT)'ROOT NOT FOUND IN XTEMP'
```

C

```
XION=DUMMY(8)
EAF=DUMMY(9)
EFV=DUMMY(10)
HOLES=DUMMY(11)
```

C

```
VDIFF=BRRIER-EFV
```

C

```
RETURN
END
```

```

10 / 17 / 1981      11 : 57 : 28      EQU.GV

FUNCTION EQU(EIF,DUMMY)
C
C   DIMENSION DUMMY(11)
EGAP=DUMMY(1)
EIF=DUMMY(2)
ENSUBI=DUMMY(3)
T=DUMMY(4)
BOLTZ=DUMMY(5)
BARRIER=DUMMY(6)
ACCPTR=DUMMY(7)
C
EFV=EIF-EIF
EAF=4.38D-2-3.037D-8*ACCPTR*(1.0/3.0)-EFV
XION=1.0D0/(1.0+(4.0+2.0/DEXP(4.4D-2/(BOLTZ*T))))*DEXP(EAF/(BOLTZ*T)))
XION=XION*ACCPTR
C
HOLES=ENSUBI*DEXP(EIF/(BOLTZ*T))
EQU=(HOLES-XION)/ACCPTR
C
DUMMY(8)=XION
DUMMY(9)=EAF
DUMMY(10)=EFV
DUMMY(11)=HOLES
C
RETURN
END

```

APPENDIX 1-I

Program for Numerically Solving Poisson's Equation for a One-Dimensional
Schottky Barrier

<u>Title</u>	<u>Page</u>
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EQUILIB	233
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[illegible]

```
COMMON /COM1/ XPOS(200)
COMMON /COM2/ XDLT(200)
COMMON /COM3/ A(200,2)
COMMON /COM4/ XL(200,2)
COMMON /COM5/ U(200)
COMMON /COM6/ EDENS(200)
COMMON /COM7/ HDENS(200)
COMMON /COM8/ Q(200)
COMMON /COM9/ ITTL(200)
COMMON /COM10/ UNEW(200)

COMMON /INTGR/ JMAX, JUNCTN, NSTEP
COMMON /WRALZE/ DNSRM, PSINRM, DEBYE
COMMON /XREAL/ BRRIER, GAP, TEMP, ACCTPR, VDIFF, VAPPL0, VAPPL
      , ENSUB1, XDELT1, XDELT2, XION, VOLT, XLNGTH, XJUNCTN, BOLTZ
COMMON /IO/ LUIN, LUIN2, LUOUT, LUOUT2
```

-----INITIALIZE MISC CONSTANTS-----

```

ACCPTR=1.0D15
TEMP=7.7D1
VAPPL0=0.0D0
VDELTA=0.0D0
NSTEP=1
BARRIER=2.7D-1
LUIN=11
LUIN2=LUIN
LUOUT=10

```

```

LUOUT2=LUOUT
-----CALCULATE EQUILIB. CHARACTERISTICS OF SI AT TEMP-----
CALL EQUILIB
-----NORMALIZE ALL PARAMETERS-----
CALL NRMLIZ
=====
TOP OV VOLTAGE STEPPING LOOP
=====
NCOUNT=1
VAPPL=VAPPL0-VDELT
20 CONTINUE
VAPPL=VAPPL+VDELT
CALL GRID
CALL LMATRIX
CALL INITIAL
CALL HOLES
CALL CHARGE
CALL PICARD
NCOUNT=NCOUNT+1
IF (NCOUNT.GT.NSTEP) GOTO 30
CALL OUTPUT
GOTO 20
30 CONTINUE
STOP

```

4
*
7
1
3
2

END

C C C

EQUILIB.GV

7 : 3 : 53

10 / 21 / 1981

SUBROUTINE EQUILB

```

=====
      USING UNNORMALIZED VARIABLES. CALCULATES THE TEMPERATURE-
      DEPENDENT BAND GAP, THE IONIZED ACCEPTOR DENSITY, AND THE BUILT-IN
      POTENTIAL BARRIER, ACCOUNTING FOR THE TEMPERATURE DEPENDENCE OF
      THE INTRINSIC DENSITY AND OF THE FERMI LEVEL.
=====

```

ORIGINAL:D.P. KENNEDY SASSOC., GAINESVILLE FLA.

```

=====
      COMMON /COM1/ XPOS(200)
      COMMON /COM2/ XDIT(200)
      COMMON /COM3/ A(200,2)
      COMMON /COM4/ XL(200,2)
      COMMON /COM5/ U(200)
      COMMON /COM6/ EDENS(200)
      COMMON /COM7/ HDENS(200)
      COMMON /COM8/ Q(200)
      COMMON /COM9/ ITTL(200)
      COMMON /COM10/ UNCW(200)

      COMMON /INTGR/ JMAX, JUNCTN, NSTEP
      COMMON /NRMLZE/ DMSHRM, PSINRM, DEBYE
      COMMON /XREAL/ BARRIER, GAP, TEMP, ACCTR, VDIFF, VAPPL0, VAPPL
      &, EMSUB1, XDILT1, XDILT2, XION, VOLT, XLNGTH, XJUNCTN, BOLTZ
      COMMON /IO/ LUIN, LUIN2, LUOUT, LUOUT2

```

```

      NDOPE=0.000
      T=TEMP/3.D2
      BOLTZ=0.02585*T
      EGAP=1.165-7.242D-3*T-3.664D-2*T+T
      EIV=EGAP/2.D0-1.306D-2*T
      X=EIV
      KEY=1
      GO TO 170

```


LEVEL 10-UV

```
100 VDIFF=BARRE-EFV
   WRITE(LUOUT2,1000)TEMP,EGAP,EIV,EIF,EFV,ENSUBI,XION,VDIFF
1000 FORMAT(2X,/,3X,TEMP,5X,EGAP,7X,EIV,7X,EIF,7X,EFV,
   36X,ENSUBI,4X,XION,4X,VDIFF,/,1X,1P8E10.2,/)
   RETURN
   END
```

2 1

NRMLIZ.GV

7 : 5 : 27

10 / 21 / 1981

SUBROUTINE NRMLIZ

SUBROUTINE NRMLIZ IS USED TO NORMALIZE FREQUENTLY USED
PARAMETERS FOR THE ANALYSIS OF A
SCHOTTKY BARRIER ON P-TYPE SILICON

COMMON /COM1/ XPOS(200)
COMMON /COM2/ XDLT(200)
COMMON /COM3/ A(200,2)
COMMON /COM4/ XL(200,2)
COMMON /COM5/ U(200)
COMMON /COM6/ EDENS(200)
COMMON /COM7/ HDENS(200)
COMMON /COM8/ Q(200)
COMMON /COM9/ IITL(200)
COMMON /COM10/ UNEW(200)

COMMON /INTGR/ JHAX, JUNCTN, NSTEP
COMMON /NRMLZE/ DNSNRH, PSINRM, DEBYE
COMMON /XREAL/ BARRIER, GAP, TEMP, ACCPTR, VDIFF, VAPPL0, VAPPL
8, ENSUBI, XDELT1, XDELT2, XION, VDLT, XLNGTH, XJUNCTN, BOLTZ
COMMON /IO/ LUIN, LUIN2, LUOUT, LUOUT2

DNSNRH=XION
PSINRM=BOLTZ
DEBYE=DSORT(11.7*8.85D-14*BOLTZ/(1.6D-19*XION))
TEMPNRH=3.0D2

VAPPL0=VAPPL0/PSINRM
VDLT=VDLT/PSINRM
VDIFF=VDIFF/PSINRM
XLNGTH=XLNGTH/DEBYE
XJUNCTN=XJUNCTN/DEBYE
XION=XION/DNSNRH

RETURN
END

```

10 / 21 / 1981          7 : 6 : 18          GRID.GV
SUBROUTINE GRID
=====
SUBROUTING GRID SETS UP LATTICE PARAMETERS FOR THE FINITE DIFF.
ARRAYS
=====
COMMON /COM1/ XPOS(200)
COMMON /COM2/ XDLY(200)
COMMON /COM3/ A(200,2)
COMMON /COM4/ XL(200,2)
COMMON /COM5/ U(200)
COMMON /COM6/ EDENS(200)
COMMON /COM7/ HDENS(200)
COMMON /COM8/ Q(200)
COMMON /COM9/ ITTL(200)
COMMON /COM10/ UNEW(200)

COMMON /INTGR/ JMAX, JUNCTN, NSTEP
COMMON /NRMLZE/ DNSNRN, PSINRM, DERVE
COMMON /XREAL/ BRRIER, GAP, TEMP, ACCTR, VDIFF, VAPPL0, VAPPL
&, ENSUB1, XDELT1, XDELT2, XION, VDLY, XLNGTH, XJUNCTN, BOLTZ
COMMON /IO/ LUIN, LUIN2, LUOUT, LUOUT2

WRITE(LUOUT2) 'SUBROUTINE GRID'

-----CALC LENGTH OF SI REGION-----
UD=DSORT(2.000*(VAPPL+VDIFF)/XION)
UD=1.500*UD

XJUNCTN=UD*1.00-1
XLNGTH=UD*1.100

-----SET GRID SPACING-----
JMAX=UD
IF (JMAX.LT.100) JMAX=200

```

```

JUNCTN=JMAX/10
XDELT1=1.000
XDELT2=1.000

```

```

-----PTSI REGION-----

```

```

SUM=1.000
JMAXX=JUNCTN-2
DO 10 J=1,JMAXX
SUM=SUM+XDELT1**J
10 CONTINUE

```

```

XDELT(I)=XJUNCTN/SUM
JMAXX=JUNCTN-1
DO 20 I=1,JMAXX
XDELT(I+1)=XDELT(I)*XDELT1
20 CONTINUE

```

```

XPOS(1)=0.000

```

```

DO 30 J=2,JUNCTN
XPOS(J)=XPOS(J-1)+XDELT(J-1)
30 CONTINUE

```

```

----- SILICON REGION -----

```

```

SUM=1.000
JMAXX=JMAX-JUNCTN-1
DO 40 J=1,JMAXX
SUM=SUM+XDELT2**J
40 CONTINUE

```

```

XDELT(JMAX-1)=40/SUM
JMAXX=JMAX-JUNCTN
DO 50 K=2,KMAXX
J=JMAX-K
XDELT(J)=XDELT(J+1)*XDELT2
50 CONTINUE

```

```

JMINN=JUNCTN+1

```

```
DO 60 J=JMIN,JMAX  
  XPOS(J)=XPOS(J-1)+XDLT(J-1)  
60 CONTINUE
```

C

```
  RETURN  
  END
```

LMATRIX.GV

7 : 7 : 37

10 / 21 / 1981

```

=====
SUBROUTINE LMATRIX SETS UP THE FINITE-DIFFERENCE MATRIX FOR SOLVING
.      POISSON'S EQUATION. THEREAFTER THIS MATRIX IS
.      SUBJECTED TO A CHOLESKY DECOMPOSITION YIELDING
.      A LOWER DIAGONAL L MATRIX.
=====

```

ORIGINAL: D.P. KENNEDY & ASSOC., GAINESVILLE FLA.

SUBROUTINE LMATRIX

```

COMMON /COM1/ XPOS(200)
COMMON /COM2/ XDLT(200)
COMMON /COM3/ A(200,2)
COMMON /COM4/ XL(200,2)
COMMON /COM5/ U(200)
COMMON /COM6/ EDENS(200)
COMMON /COM7/ HDENS(200)
COMMON /COM8/ Q(200)
COMMON /COM9/ ITTL(200)
COMMON /COM10/ UNEW(200)

```

```

COMMON /INTGR/ JMAX, JUNCTN, NSTEP
COMMON /NRHLZE/ DNSRNM, PSINRM, DEBYE
COMMON /XREAL/ BARRIER, GAP, TEMP, ACPTIR, VDIFF, VAPPL0, VAPPL
&, ENSUBI, XDDEL1, XDDEL2, XION, VOLT, XLNGTH, XJUNCTN, BOLTZ
COMMON /IO/ LUIN, LUIN2, LUOUT, LUOUT2

```

----- SET UP MATRIX FOR POISSONS EQUATION -----

```

A(1,1)=0.0
A(1,2)=(XDLT(1)+XDLT(2))/(XDLT(1)+XDLT(2))
K=0.000

```

```

JMAXX=JMAX-2
DO 1 J=2,JMAXX

```

```

C C C
A(J,1)=-1.000/XDLT(J)
A(J,2)=(XDLT(J)+XDLT(J+1))/(XDLT(J)+XDLT(J+1))
1 CONTINUE
C C C
XDL1=1.000
ID2=0
N=JMAX-2
M=1
DO 70 I=1,N
  IP=M-I+1
  IF (1.0T.M) IP=0
  IR=I-M+IP
C
DO 60 J=IP,M
  IX=J-1
  IQ=M-J+IP
  JJ=J+1
  Y=A(I,JJ)
  DO 10 K=IP,IX
    KK=K+1
    IQ=IQ+1
    Y=Y-XL(I,KK)*XL(IR,IQ)
    IQ=IQ+1
  10 CONTINUE
C
  IF (J.NE.M) GOTO 50
  XDL1=XDL1*Y
C
  IF (Y.NE.0.000) GOTO 30
  ID2=0
  GOTO 9998
C
20 CONTINUE
  IF (DABS(XDL1).LT.1.000) GOTO 30
  XDL1=XDL1*0.0625
  ID2=ID2+4
  GOTO 20

```

```

C      30 CONTINUE
      IF (DABS(XD1).GE.0.0625) GOTO 40
      XD1=XD1*16.0D0
      ID2=ID2-4
      GOTO 30
C
      40 CONTINUE
C
      IF (Y.LI.0.0D0) GOTO 9999
      JJ=J+1
      XL(I,JJ)=1.0D0/DSQRT(Y)
      GOTO 60
C
      50 CONTINUE
      JJ=J+1
      MM=M+1
      XL(I,JJ)=Y*XL(IR,MM)
      IR=IR+1
C      60 CONTINUE
C
      RETURN
C
      9998 CONTINUE
      STOP Y=0
C
      9999 CONTINUE
      STOP Y<0
C
      END

```

1975-76

—
—
==
C
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—

INITIAL-60

741111 3N11003575
SUBROUTINE INITIAL

```
=====
SUBROUTINE INITIAL IS USED TO INITIALIZE ARRAYS PRIOR TO
ENTERING PICARD AND UNDERTAKING AN
ITERATIVE SOLUTION FOR THE SCHOTTKY
BARRIER PROBLEM
=====
```

ORIGINAL: D.F. KENNEDY & ASSOC., GAINESVILLE, FLA.

COMMON /COM1/ XPOS(200)
COMMON /COM2/ XDLT(200)
COMMON /COM3/ A(200,2)
COMMON /COM4/ XL(200,2)
COMMON /COM5/ U(200)
COMMON /COM6/ EDEWS(200)
COMMON /COM7/ HDEWS(200)
COMMON /COM8/ Q(200)
COMMON /COM9/ ITTL(200)
COMMON /COM10/ UNCH(200)

```
COMMON /INTEGR/ JMAX, JUNCTN, NSTEP
COMMON /NRMALZE/ DSNRM, PSINRM, DEBYE
COMMON /XREAL/ BRRIER, GAP, TEMP, ACCTPR, VDIFF, VAPFLQ, VAPPL
COMMON /XENSUBI/ XDEL1, XDEL2, XEN, VOL1, XLNGTH, XJUNCTN, BOLIZ
COMMON /IO/ LUIN, LUIN2, LCUOUT, LCUOUT2
```

----- CALCULATE DEPLETION LAYER WIDTH -----
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99
100

```
HFD=DSORT(C=DD04(=APP1+UNDEF) / (NOIYN)
```

----- INITIALIZE METAL POTENTIAL -----

```
DO 10 J=1,JUNCTN
  U(J)=VAPFL+VDIFF
10 CONTINUE
```


10 2 1981 7 2 16 HOLES.GV

SUBROUTINE HOLES

=====

SUBROUTINE HOLES IS USED TO CALCULATE THE HOLE DENSITY

WITHIN A P-TYPE SPOTTY BARRIER

=====

ORIGINAL: D.P. KENNEDY & ASSOC., GAINESVILLE, FLA.

=====

COMMON /COM1/ XPOS(200)

COMMON /COM2/ XDLT(200)

COMMON /COM3/ A(200,2)

COMMON /COM4/ XL(200,2)

COMMON /COM5/ U(200)

COMMON /COM6/ EDENS(200)

COMMON /COM7/ HDENS(200)

COMMON /COM8/ G(200)

COMMON /COM9/ ITTL(200)

COMMON /COM10/ UNEW(200)

COMMON /INTGR/ JMAX, JUNCTN, NSTEP

COMMON /NRNLZE/ DNSNRM, PSIPRM, DEBYE

COMMON /XREAL/ BARRIER, GAP, TEMP, ACPTFR, VDIFF, VAPPL0, VAPPL

S, ENSURI, XDEL11, XDEL12, XION, UDLT, XLNGTH, XJUNCTN, BOLTZ

COMMON /IG/ LUIN, LUIN2, LUOUT, LUOUT2

----- CALCULATE HOLE DENSITY DISTRIBUTION -----

HDENS(JMAX)=XION

KMAX=JMAX-JUNCTN

DO 10 K=1, KMAX

J=JMAX-K

UDLT=U(J)-U(J+1)

IF (UDLT.GT.1.0D2) UDLT=1.0D2

IF (UDLT.LT.-0.000) UDLT=0.000

IF (HDENS(J+1).LE.1.0D-30) UDLT=0.000

IF (HDENS(J+1).GT.1.0D30) UDLT=0.000

HDENS(J)=HDENS(J+1)+DEXP(-UDLT)

```

C      TYPE J,HDEMS(J)
      IF(HDEMS(J).LE.1.0D-50) HDEMS(J)=1.0D-50
      10 CONTINUE
C
C      RETURN
C
C      END

```

CHARGE.GV

7 : 11 : 14

12 / 21 / 1981

SUBROUTINE CHARGE

=====

SUBROUTINE CHARGE: IS USED TO CALCULATE THE ELECTROSTATIC
CHARGE DISTRIBUTION THROUGHOUT THE
ONE-DIMENSIONAL SCHOTTKY BARRIER.

=====

ORIGINAL: D.P. KENNEDY & ASSOC., GAINESVILLE, FLA

=====

COMMON /COM1/ XPOS(200)
COMMON /COM2/ XDLT(200)
COMMON /COM3/ AC(200,2)
COMMON /COM4/ XL(200,2)
COMMON /COM5/ U(200)
COMMON /COM6/ EDENS(200)
COMMON /COM7/ HDENS(200)
COMMON /COM8/ Q(200)
COMMON /COM9/ ITTL(200)
COMMON /COM10/ UNEW(200)

COMMON /INTGR/ JMAX,JUNCTN,NGSTEP
COMMON /RMLZE/ SNSMRM,PSINRM,DEBYE
COMMON /XREAL/ SRRIEF,GAP,TEMP,ACCPTR,VDIFF,VAPPLQ,VAPPL
&,ENSUBI,XDELT1,XDELT2,XION,VDLT,XLENGTH,XJUNCTN,BOLTZ
COMMON /IO/ LUIN,LUIN2,LUOUT,LUOUT2

----- METALLIC REGION -----

Q(1)=(VAPPL+VDIFF)/XDLT(1)

DO 10 J=2,JUNCTN
Q(J)=0.000
10 CONTINUE

----- ZERO EDENS ARRAY -----

```

DO 20 J=1,NBY
  EDENS(J)=0.000
20 CONTINUE

----- SILICON REGION -----

SUM=0.000
JMIN=JUNCTN+1
JMAX=JMAX-I
DO 30 J=JMIN,JMAX
  Q0=-(XION-HDENS(J)+EDENS(J))
  Q1=-(XION-HDENS(J+1)+EDENS(J+1))
  SUM=SUM+((Q1+Q0)/2.000)*XDLT(J)
  Q(J)=Q0*(XDLT(J-1)+XDLT(J))/2.000
30 CONTINUE
Q(JMAX-2)=-((HAPPL+VDIFF)/XDLT(JMAX-1))
Q(JUNCTN)=-SUM*(XDLT(JUNCTN-1)+XDLT(JUNCTN))/2.000
Q(JUNCTN)=Q(JUNCTN)+1.0710

RETURN
END

```

10 / 20 / 1981 7 : 12 : 22 PICARD.SV

```

SUBROUTINE PICARD
=====
C
C
C SUBROUTINE PICARD: IS THE ADMINISTRATION PROGRAM FOR A
C . PICARD ITERATION BETWEEN POISSON S
C . EQUATION AND THE HOLE DISTRIBUTION.
C
C
C
C
C ORIGINAL: D.P. KENNEDY & ASSOC., GAINESVILLE, FLA.
C
C
C
C
C COMMON /COM1/ XPOS(200)
C COMMON /COM2/ XDLT(200)
C COMMON /COM3/ A(200,2)
C COMMON /COM4/ XL(200,2)
C COMMON /COM5/ U(200)
C COMMON /COM6/ EDENS(200)
C COMMON /COM7/ HDENS(200)
C COMMON /COM8/ Q(200)
C COMMON /COM9/ ITTL(200)
C COMMON /COM10/ UNEW(200)
C
C COMMON /INT1/ JMAX, JUNCTN, NSTEP
C COMMON /NRMLZE/ BNSNRN, PSINRM, DERYE
C COMM.N /XREAL/ BRRIER, GAP, TEMP, ACCPTR, UDIFF, VAPPL3, VAPPL
C, ENSUB1, XDILT1, XDILT2, XION, VDLT, XLNGTH, XJUNCTN, BOLTZ
C COMMON /IO/ LUIN, LUIN2, LUOUT, LUOUT2
C
C I=0
C N=1
10 CONTINUE
C
C CALL POISSN
C
C -----CALC MAX UDELT-----
C
C JJ=0
C UDELT=0.000
C JMAXX=JMAX-1

```

```

DO 20 J=2,JMAX
R=UNEW(J)-U(J)
IF(DABS(R).LT.DABS(UDEL)) GOTO 20
JJ=J
UDEL=R
20 CONTINUE
C
P=UDEL*PCINRM
C
IF(DABS(P).LE.1.0D-4) GOTO 40
C
C-----UNDER RELAX POTENTIAL-----
C
URELAX=0.15D0
JMAXX=JMAX-1
GO 30 J=2,JMAX
U(J)=U(J)+URELAX*(UNEW(J)-U(J))
30 CONTINUE
C
CALL RESID(RESMX)
C
CALL HOLES
CALL CHARGE
N=N+1
I=I+1
GOTO 10
C
40 CONTINUE
C
RETURN
END

```

```

12 / 21 / 1981          7 : 13 : 27          POISSN.GV
=====
SUBROUTINE POISSN: IS USED TO SOLVE POISSON'S EQUATION FOR
A ONE DIMENSIONAL SCHOTTKY BARRIER. THIS
CALCULATION IS BASED UPON THE SECOND STEP
OF THE CHOLOSKY TECHNIQUE FOR THE SOLUTION
OF THE MATRIX EQUATION.
=====
ORIGINAL: D.P. KENNEDY & ASSOC., GAINESVILLE, FLA.
=====
SUBROUTINE POISSN
COMMON /COM1/ XPOS(200)
COMMON /COM2/ XDLT(200)
COMMON /COM3/ A(200,2)
COMMON /COM4/ XL(200,2)
COMMON /COM5/ U(200)
COMMON /COM6/ EDENS(200)
COMMON /COM7/ HDENS(200)
COMMON /COM8/ Q(200)
COMMON /COM9/ ITTL(200)
COMMON /COM10/ UNEQ(200)

COMMON /INTOR/ JMAX,JUNCTN,NSTEP
COMMON /NRMLZE/ DMSNRM,PSINRM,DEBYE
COMMON /XREAL/ BRIER,GAP,TEMP,ACCPTR,VDIFF,VAPPL0,VAPPL
& ENSUBT,XDELT1,XDELT2,XION,VOLT,XLENGTH,XJUNCTN,BOLTZ
COMMON /IO/ LUIN,LUIN2,LUOUT,LUOUT2

WRITE(LUOUT2)'SUBROUTINE POISSN'

N=JMAX-2
M=1
IS=M-1

DO 20 I=1,N

```

```

IP=0
IF (I.LE.0) IP=M-I+1
IQ=I
Y=Q(I)

C
KMAX=IS+1-IP
DO 10 KK=1,KMAX
K=IS+1-KK
IQ=IQ+1
JK=K+1
Y=Y-XL(I,K)*UNEQ(IQ+1)
10 CONTINUE

C
MM=M+1
UNEQ(I+1)=Y*XL(I,MM)

C
20 CONTINUE
DO 40 IX=.N
I=N+1-IX
IP=0
IF (N-I.LE.M) IP=M-N+I
Y=UNEQ(I+1)
IQ=I

C
KMAX=IS+1-IP
DO 30 KK=1,KMAX
K=IS+1-KK
IQ=IQ+1
JK=K+1
Y=Y-XL(I,K)*UNEQ(IQ+1)
30 CONTINUE

C
MM=M+1
UNEQ(I+1)=Y*XL(I,MM)

C
40 CONTINUE

C
RETURN
END
C
C

```

RESID.GV

7 : 14 : 40

10 / 21 / 1981

SUBROUTINE RESID (RESH)

 SUBROUTINE RESID: IS USED TO CALCULATE THE RESIDUALS
 . ARISING FROM A CHOLOSKY SOLUTION OF
 . POISSON'S EQUATION. THESE RESIDUALS
 . ARE STORED IN THE Q(J) ARRAY AND THE
 . MAXIMUM RESIDUAL PASSED TO THE CALLING
 . SUBROUTINE.

ORIGINAL: D.P. KENNEDY & ASSOC., GAINESVILLE, FLA.

 COMMON /COM1/ XPOS(200)
 COMMON /COM2/ XDLT(200)
 COMMON /COM3/ A(200,2)
 COMMON /COM4/ XL(200,2)
 COMMON /COM5/ U(200)
 COMMON /COM6/ EDENS(200)
 COMMON /COM7/ HDENS(200)
 COMMON /COM8/ Q(200)
 COMMON /COM9/ ITTL(200)
 COMMON /COM10/ UNEW(200)

COMMON /INTGR/ JMAX, JUNCTN, NSTEP
 COMMON /NRMLZE/ DSENRN, PSINRM, DEBYE
 COMMON /XREAL/ BRKIER, GAP, TEMP, ACCTR, VDIFF, VAPPL0, VAPPL
 &, ENSUR1, XDELT1, XDELT2, XION, VDLT, XLNGTH, XJUNCTN, BOLTZ
 COMMON /IO/ LUIN, LUIN2, LUOUT, LUOUT2

RESHX=0.000

----- CALCULATE RESIDUAL -----

R=Q(1)-A(1,2)*UNEW(2)-A(2,1)*UNEW(3)

```

RR=D1AX1(DABS(R),RESMX)
IF(RR.GT.RESMX) RESMX=RR

```

C

```

JMAXX=JMAX-3
DO 10 J=2,JMAXX
R=Q(J)-A(J,1)*UNEW(J)-A(J,2)*UNEW(J+1)-A(J+1,1)*UNEW(J+2)
RR=D1AX1(DABS(R),RESMX)
IF(RR.GT.RESMX) RESMX=RR
:0 CONTINUE

```

C

```

R=Q(JMAX-2)-A(JMAX-2,1)*UNEW(JMAX-2)-A(JMAX-2,2)*UNEW(JMAX-1)
RR=D1AX1(DABS(R),RESMX)
IF(RR.GT.RESMX) RESMX=RR

```

C
C
C
C

```

RETURN
END

```

APPENDIX II

Temperature Dependent Properties of Silicon

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Fig. 32 Energy Gap in Silicon	233
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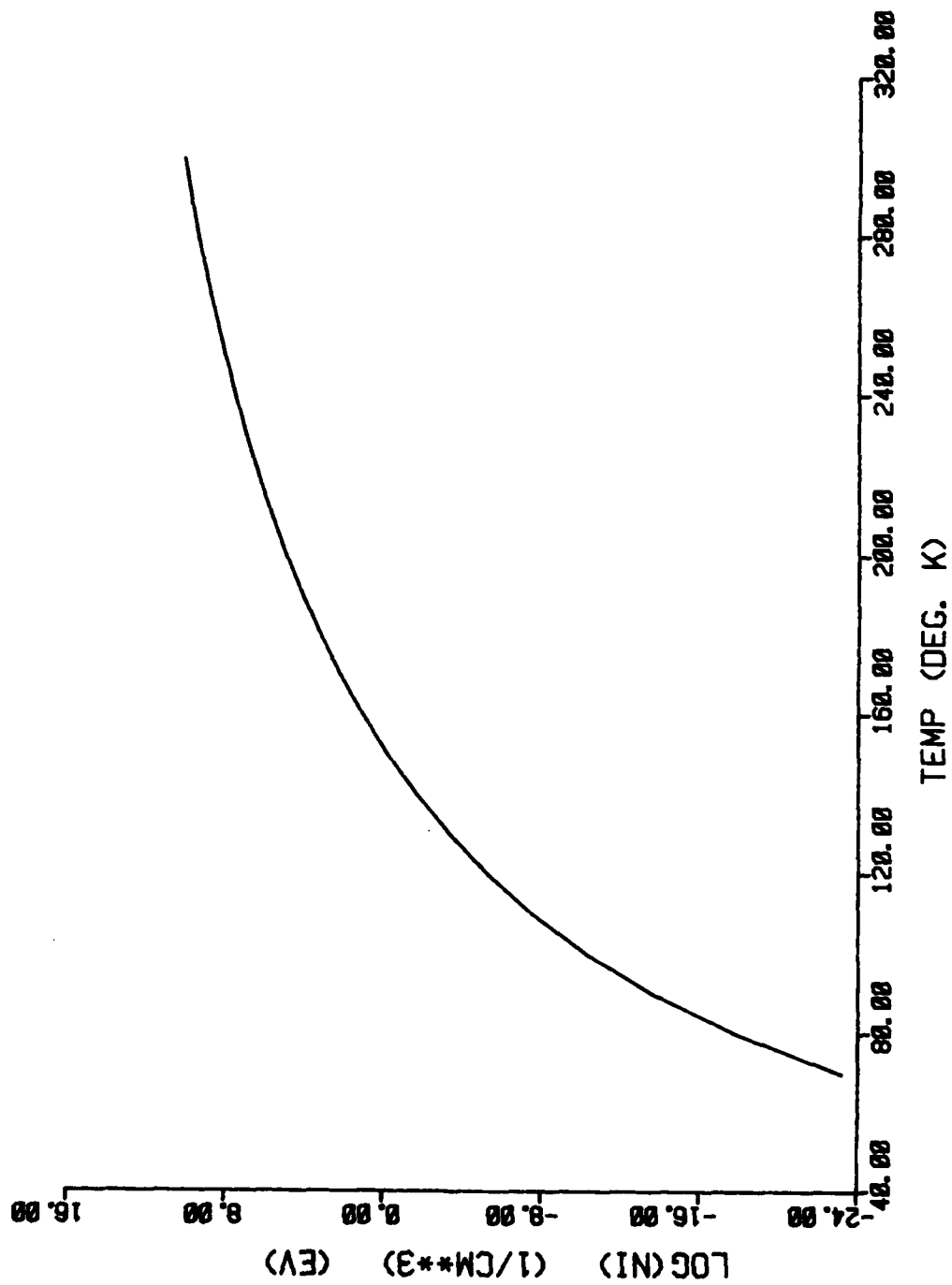


Fig. 29 Intrinsic Carrier Density in Silicon

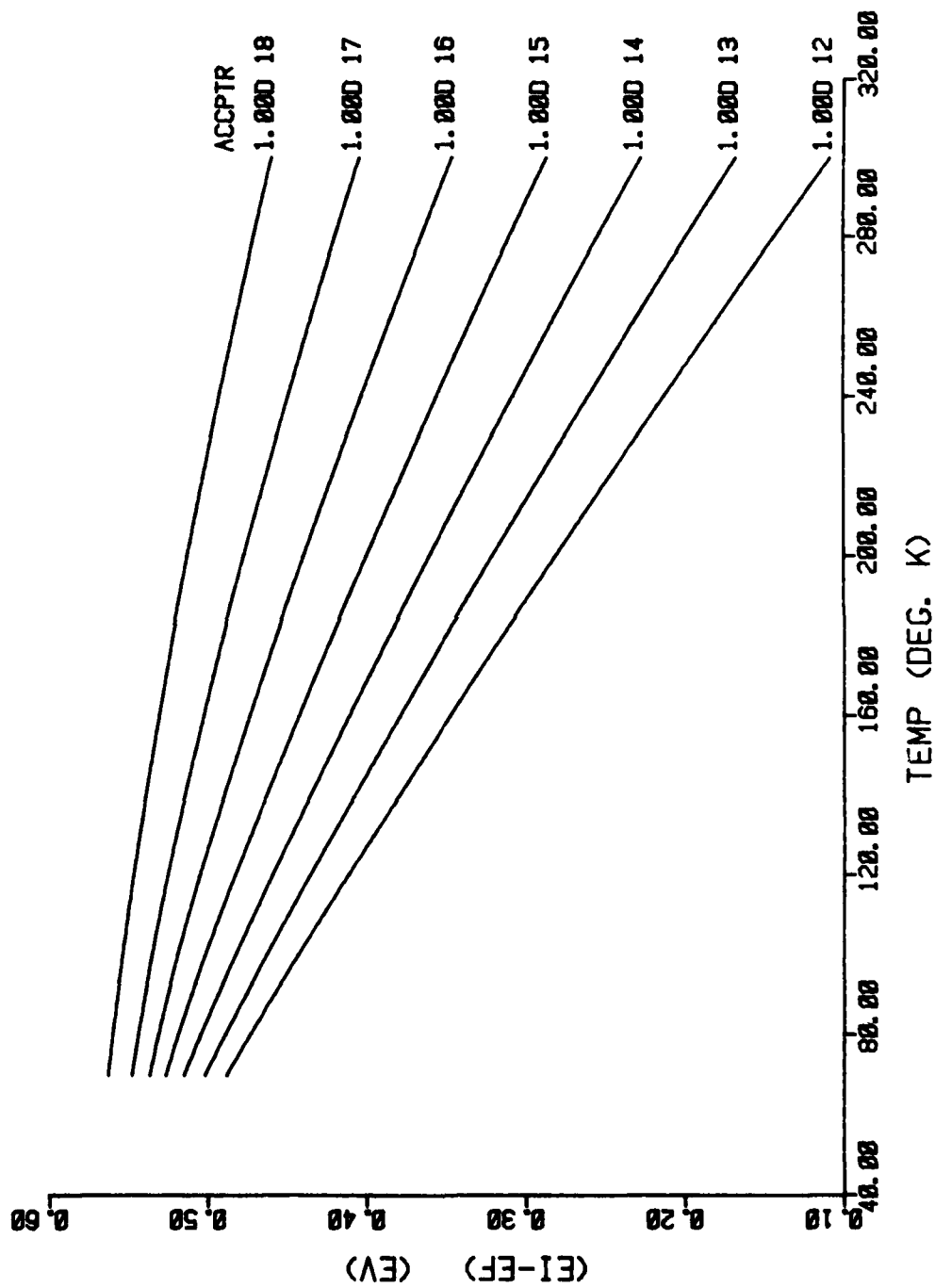


Fig. 30 $E_i - E_f$ in Silicon, Where E_i is the Intrinsic Fermi-Level and E_f is the Fermi-Level at the Specified Temperature

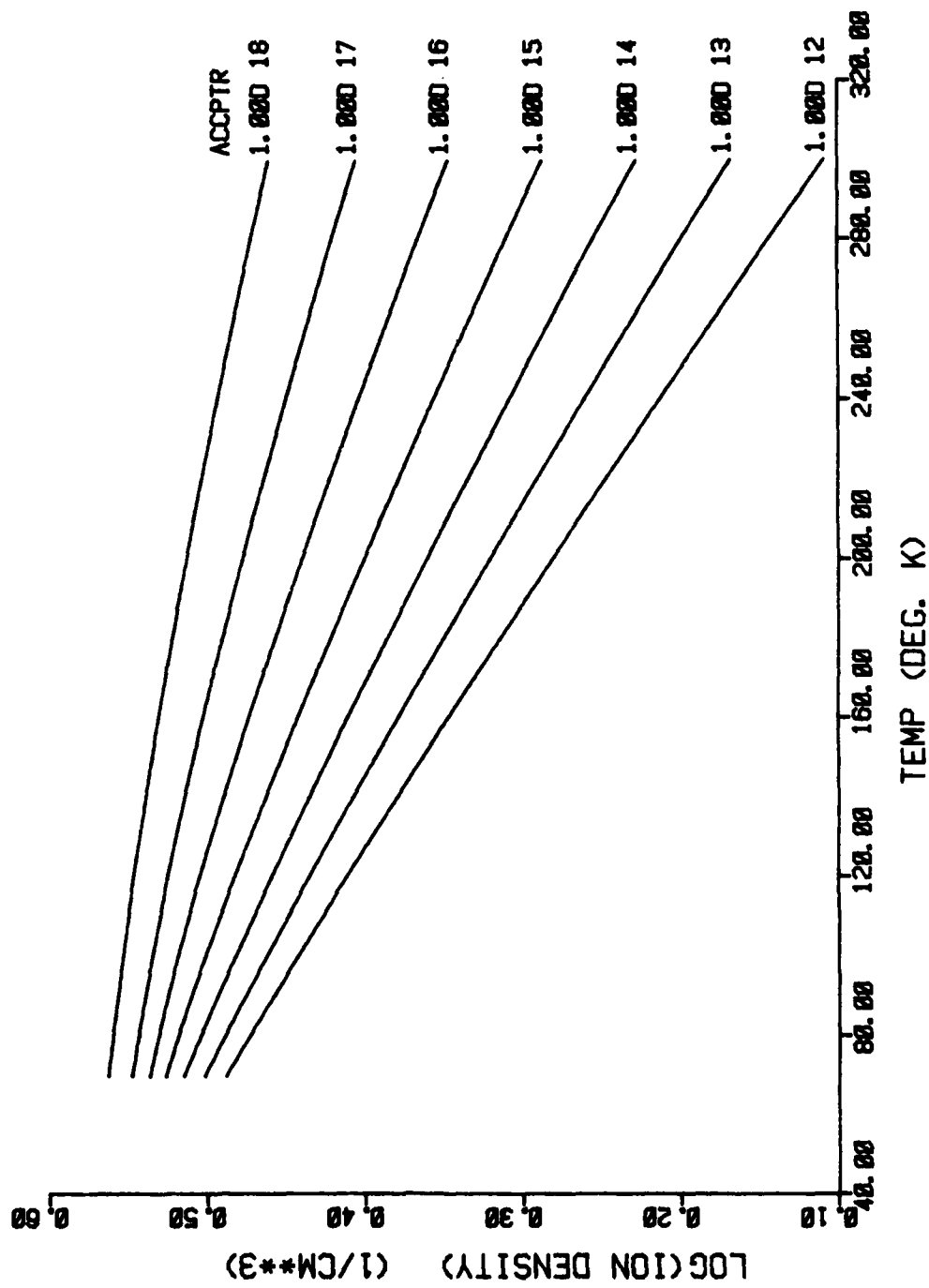


Fig.31 Ionized Impurity Atom (Boron) Density in Silicon

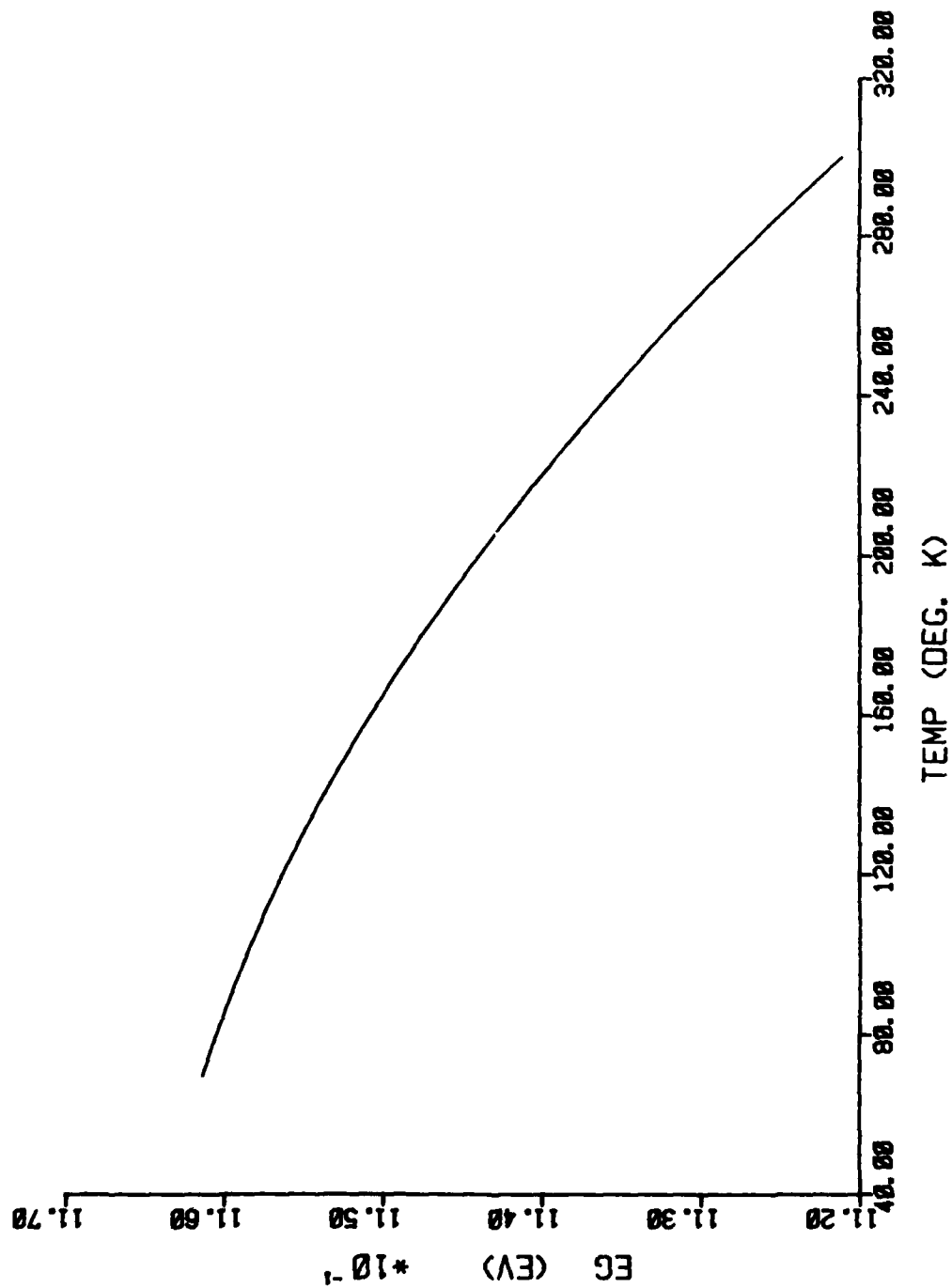


Fig.32 Energy Gap of Silicon

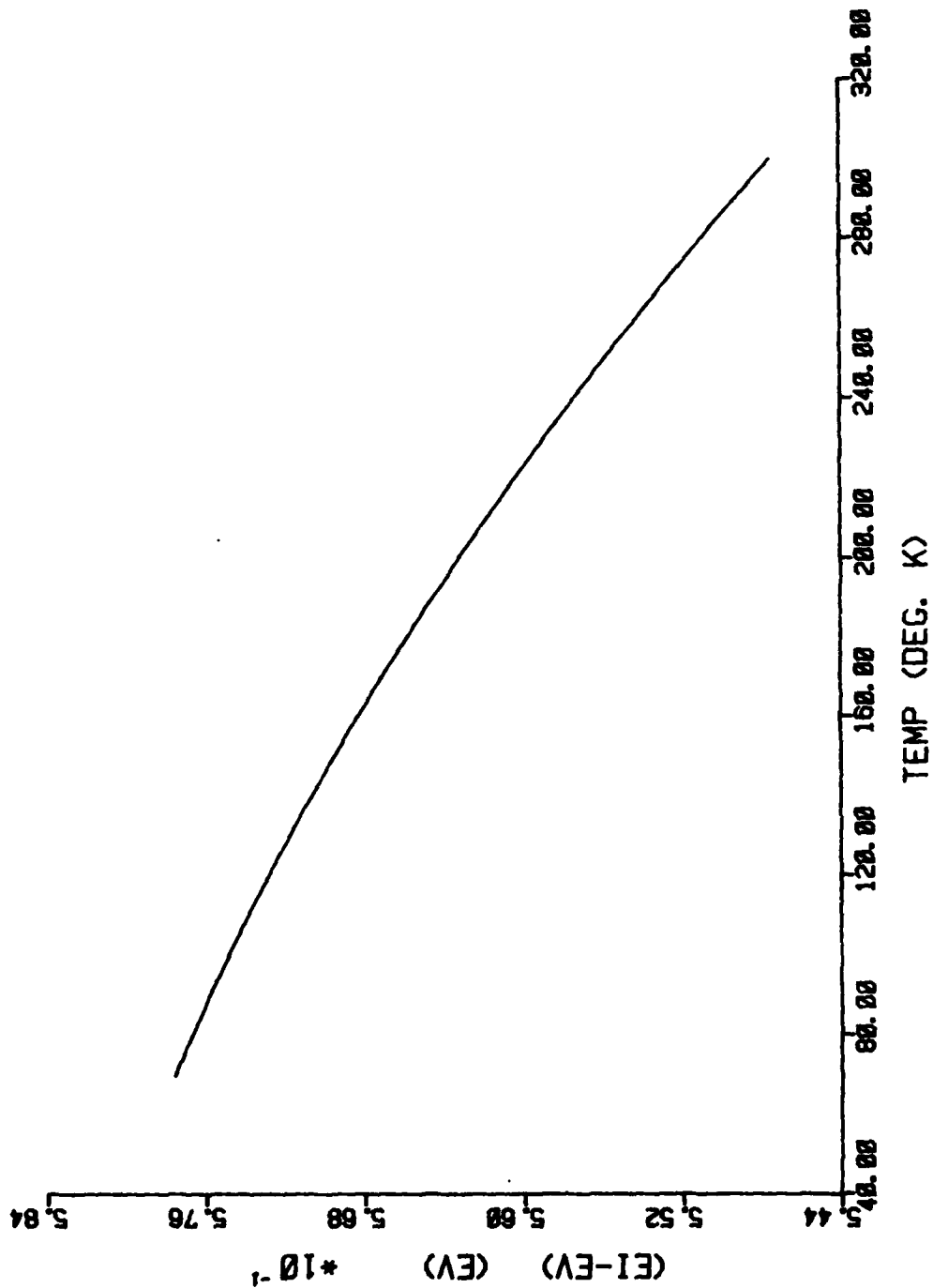


Fig.33 ($E_i - E_v$) Where in Silicon E_i is the Fermi-Level in Intrinsic Material and E_v is the Fermi-Level at the Specified Temperature

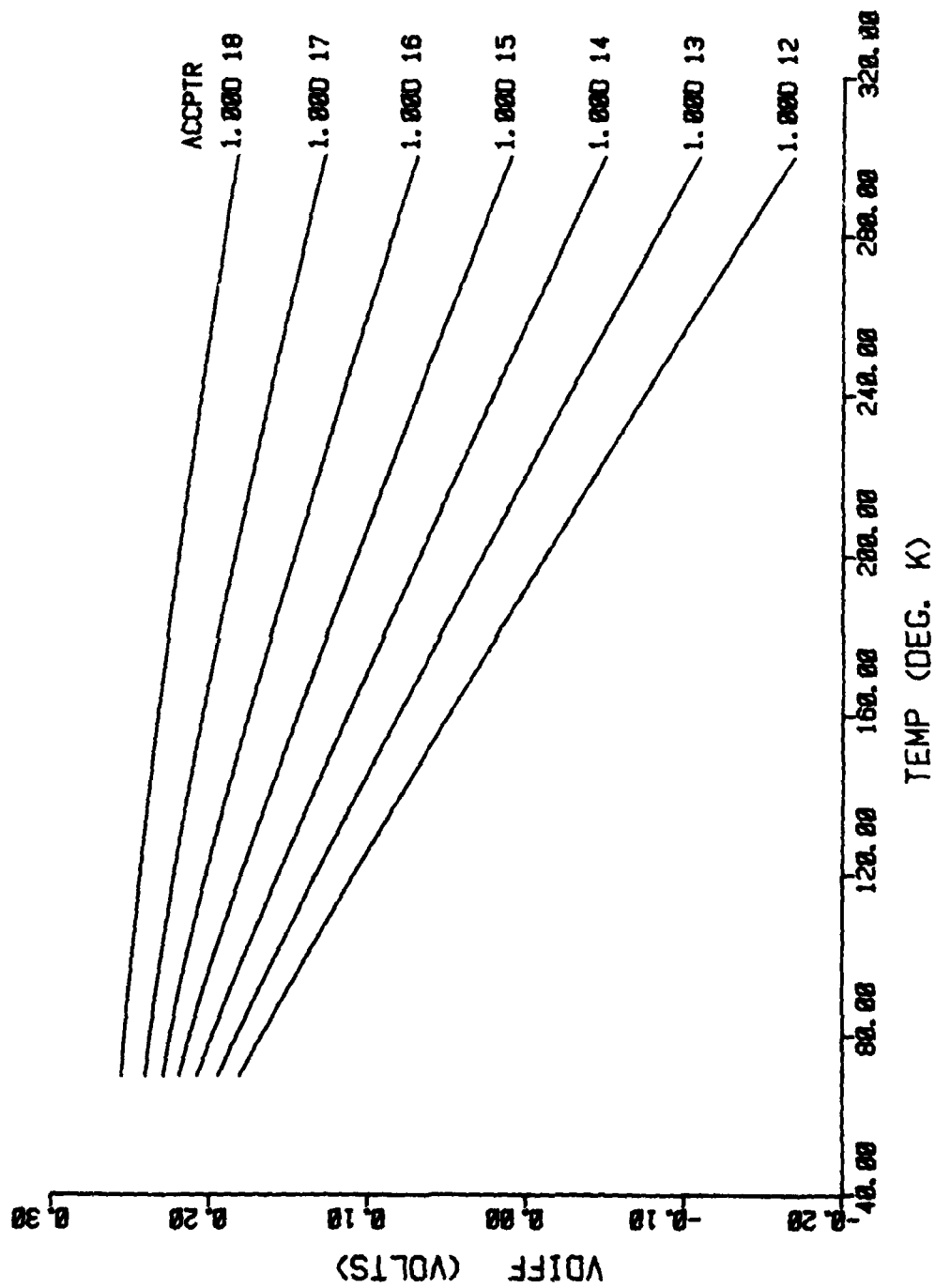


Fig.34 Diffusion Voltage in a Pt-Si Barrier Assuming a Barrier Height of 0.27 ev

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