THE EVALUATION OF E-k CURVES FROM TUNNELING CURRENTS

Thesis by

Thomas C. McGill, Jr.

In Partial Fulfillment of the Requirements

For the Degree of

Doctor of Philosophy

California Institute of Technology

Pasadena, California

1969

(Submitted May 15, 1969)

ACKNOWLEDGMENTS

I would like to express my deep indebtedness to Dr. Carver A. Mead for his constant guidance and enduring patience throughout the course of this work and the many other projects we have shared. I would like to acknowledge my gratitude to Dr. J. N. Franklin and Dr. G. W. Lewicki for providing assistance essential to the completion of this work. The financial support of both the National Science Foundation and the Hughes Aircraft Company is gratefully acknowledged. Finally, I would also like to express my gratitude to my wife, Toby, whose constant support throughout the preparation of this manuscript has made it possible, and to Dr. C. H. Wilts whose careful reading of the manuscript has resulted in improvements in both the style and clarity of this thesis.

ABSTRACT

The basis for interpreting I-V data taken on metal-insulator-metal structures with insulator thicknesses of less than 100 Å is examined carefully. A set of experimental tests for determining the applicability of the equation linking the I-V data to the E-k curve is presented. These tests are found to be a stringent requirement on the experimental data and to support strongly the interpretation of the experimental I-V in terms of the E-k curve for the insulator. A numerical technique for obtaining the E-k curve from I-V data is presented, and applied to data taken on Al-AlN-(Mg,Au) structures where it allows the evaluation of the E-k curve for AlN throughout the forbidden gap.

I. INTRODUCTION

The study of the character of electronic wavefunctions for energies in the forbidden gap of insulators[1-4] and semiconductors[5-8] by examining tunneling currents in metal-insulator-metal (MIM) and metal-semiconductor (MS) structures is currently of much interest. The dominant characteristic of these wavefunctions is the rate at which they are exponentially attenuated with distance. This rate is described by an attenuation constant k; the variation of k with electron energy is described by the E-k curve. The E-k curve is a fundamental property of the single electron states in an insulator or semiconductor; consequently, it is useful in characterizing the nature of the material.

When a crystalline insulator or semiconductor is used in these studies, the measured E-k curve is a portion of the energy band structure for complex k.[9-12]* Thus, an accurate measurement of the E-k curve presents the opportunity for a detailed comparison of the theoretical band structure with experimental data.

Some of the insulators used in these tunneling studies are disordered (possessing no well-defined crystalline lattice). In these cases the E-k curve does not correspond to a complex band structure since in a strict sense none exists. However, recent calculations by Fletcher[13,14] using the Greenian formalism introduced by Phariseau and Ziman[15]

*This is strictly true only if the presence of the metal electrodes does perturb significantly the periodic potential of the lattice. Only spatially varying potentials need be considered since a uniform potential only changes the zero of the energy. The size of these perturbing spatially varying potentials cannot be reliably estimated since the nature of the metal-semiconductor or metal-insulator interface is not completely understood. However, it is surmised from a number of other experiments that the effect of these perturbing potentials is small.

indicate that a band structurelike classification of the single particle energy spectrum in disordered materials is appropriate. In this description the electron states in the forbidden gap would be described in much the same way as the electron states in the forbidden gap of crystalline material. Thus, the expression for the tunneling currents are much the same and the E-k curve calculated from the experimental I-V data is a relevant quantity in a discussion of the electronic properties of the amorphous materials.

From the discussion above it is clear why much interesthas been and is developing in obtaining E-k curves from experimental I-V data. However, several problems have prevented this program from being carried to completion on any significant number of materials. These problems are closely intertwined. The theorists on one hand are forced by the complexity of the problem to use simplified models to derive expressions for the tunneling current which rely heavily upon the experimental results both to define their regions of validity and to provide many of the parameters in the model. On the other hand, the experimentalist is faced with not only determining whether or not the I-V data he is taking is tunneling at all, but must also find if he is in the range of validity of the simplified model. This step must precede any attempt to interpret his data. However, in the past few years, this somewhat bleak situation has been changing for the better. Due to some excellent experimental studies of tunneling both in insulators and semiconductors, a somewhat phenomenological - but self-consistent - model of tunneling currents in insulators and semiconductors has been emerging. In fact, the experimental data and the somewhat phenomenological model it has

fostered makes it desirable to make real attempts at obtaining accurate E-k curves from tunneling I-V data.

In this thesis, we present a brief derivation of the above-mentioned model for the tunneling current. A detailed technique which allows the unscrambling of the E-k curve from the I-V data is presented. In addition we present a series of criteria which must be satisfied by any experimental data before it is of sufficient quality to justify attempts at obtaining the E-k. Finally, this technique is applied to the data taken by Lewicki[3,4] on Al-AlN-(Mg,Au) MIM structures, where it allows us to obtain the E-k curve for AlN throughout the forbidden gap.

II. DISCUSSION OF TUNNELING CURRENTS IN MIM STRUCTURES

Consider the MIM structures as illustrated in Fig. 1. For insulator thickness, t , less than 100 Å and for temperatures such that thermionic emission over the barrier and thermal-tunneling emission through the top of the barrier can be neglected, the dominant mechanism of current transport through the insulator region is tunneling. This tunneling current can be divided into two parts: an elastic term in which the electron tunnels without any change in energy, and an inelastic term in which the electron interacts with an elementary excitation (i.e., phonon, magnon, etc.) during the tunneling process. The inelastic contribution to the tunneling current involves the product of the tunneling probability and the coupling strength of the elementary excitation of the tunneling electron. Therefore, the relative strength of the inelastic contribution as compared to the elastic contribution is gauged by the coupling strength of the elementary excitation to the tunneling electron. In most cases this coupling strength is small; consequently, the inelastic term may be neglected in a discussion of the tunneling current and the evaluation of the E-k curve. The elastic tunneling current from metal 1 to metal 2 (see Fig. 1) in the independent particle approximation is given by the expression

$$I_{1\to 2}(V) = e\sum_{a,b} \underset{a\to b}{\text{Rate}}\, f_1(E_a)(1-f_2(E_b)) \qquad \text{(II-1)}$$

where the $\underset{a\to b}{\text{Rate}}$ is the rate of transition from state a in metal 1 to state b in metal 2. $f_1(E_a)$ is the Fermi factor for metal 1 and $f_2(E_b)$ is the Fermi factor for metal 2. The sums in Eq. II-1 are taken over

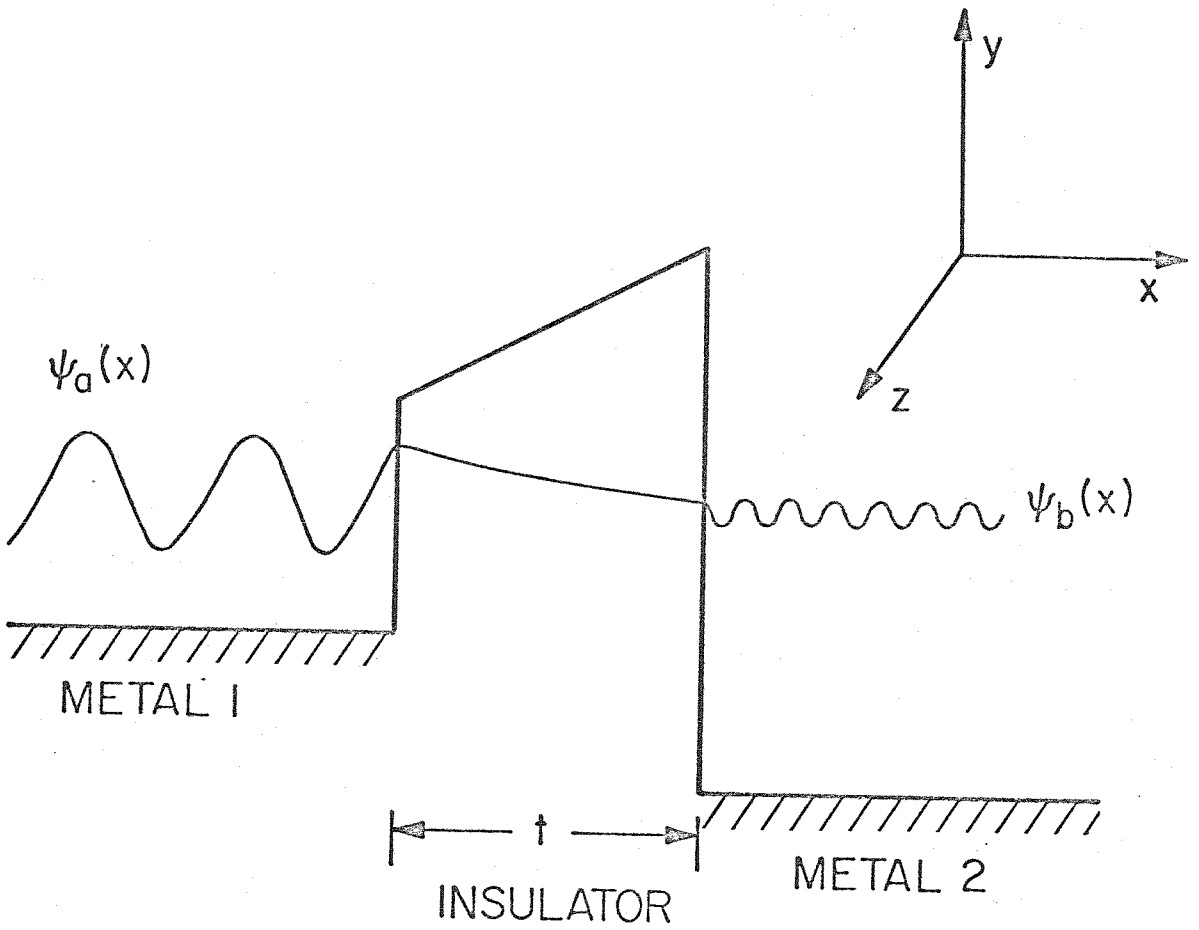

Figure 1. Schematic diagram of a metal insulator metal structure and the wavefunction of a tunneling electron.

all the states a in metal 1 which are capable of carrying charge toward the barrier and all the states b in metal 2 which are capable of carrying charge away from the barrier and have the same energy as the state a. A similar expression holds for the tunneling current from metal 2 to metal 1. Consequently, the total current is given by the expression

$$I_T(V) = e\sum_{a,b} \text{Rate}_{a\to b} f_1(E_a)(1-f_2(E_b)) - \text{Rate}_{b\to a} f_2(E_b)(1-f_1(E_a)) \qquad \text{(II-2)}$$

Time reversal invariance implies the existence of states such that $\text{Rate}_{a\to b} = \text{Rate}_{b\to a}$; therefore, we have

$$I_T(V) = e\sum_{a,b} \text{Rate}_{a\to b} (f_1(E_a)-f_2(E_b)) \qquad \text{(II-3)}$$

This is the fundamental equation to be used in discussing single particle tunneling in MIM structures. In order to proceed, definite models must be assumed for the nature of the metal and the insulator, and the dependence of the rates on the states in the metals and insulator. Henceforth, a standard model[16,17] will be used in deriving the equation used.

In the standard model the metal and insulator are assumed to be crystalline in nature. The band structure of the metals is assumed to be a single free electron-like band. The interfaces between the metal and the insulator are assumed to be sharp; specular reflection is assumed at both interfaces. Thus, we can replace the sums in Eq. II-3 by integrals over the k-space corresponding to the single bands in the metals. Thus,

$$I_T(V) = 2eV_1V_2 \int \frac{d^3k_b}{(2\pi)^3} \int \frac{d^3k_b}{(2\pi)^3} \underset{a\to b}{\text{Rate}} \; (f_1(E_a) - f_2(E_b)) \qquad \text{(II-4)}$$

where V_1 and V_2 are the volume of metal 1 and metal 2, respectively. In obtaining Eq. II-4 we have used the two-fold spin degeneracy of each state but assumed that the spin is not flipped during the transition.

Consider the rate from a to b. This rate is given by

$$\underset{a\to b}{\text{Rate}} = F_a T(a,b) \delta_{E_a,E_b} \qquad \text{(II-5)}$$

where F_a is the flux of electrons incident on the barrier in state a given that state a is occupied, and where T(a,b) is the probability of transition from state a to state b given that the electron is incident upon the barrier. δ_{E_a,E_b} is the Kronecker delta resulting from conservation of energy. The flux of electrons in state a, F_a , is given by

$$F_a = \frac{A}{V_1} v_{xa} \qquad \text{(II-6)}$$

where A is the area of the interface and v_{xa} is the component of the group velocity of an electron in state a perpendicular to the plane of the interface. (The coordinate system used throughout this discussion is shown in Fig. 1.) In principle, T(a,b) can be obtained by matching solutions of the Schrodinger equation in the insulator to state a in metal 1 and state b in metal 2. However, in practice this is much too difficult a thing to do. Nevertheless, it is possible to obtain an approximate form for the wavefunction which is very useful in determining

the nature of the transition rate.

Let us consider the form of the wavefunctions in the crystalline insulator. If we consider only the potential due to the periodic lattice of the insulator, then the usual application of Bloch's theorem[10] implies that the wavefunctions of interest in the insulator region are of the form

$$\psi_{\underset{\sim}{k},n}(\underset{\sim}{x}) = U_{\underset{\sim}{k},n}(\underset{\sim}{x}) e^{i\underset{\sim\|}{k}\cdot\underset{\sim\|}{x}} e^{ik_{x,n}(\underset{\sim\|}{k},E)x} \qquad \text{(II-7)}$$

where k_x is in general complex since the energies of the tunneling electrons lie in the forbidden gap of the insulator. $\underset{\sim\|}{x}$ denotes (y,z) and $\underset{\sim\|}{k}$ denotes (k_y,k_z). $U_{\underset{\sim}{k},n}(\underset{\sim}{x})$ is a function which has the periodicity of the lattice. The index n in Eq. II-7 labels the various solutions with energy E. When an external potential, $\varphi(x)$, which is only a function of x , is applied in the insulator region, the wavefunction can be approximated by the semiclassical approximation.* In this approximation the state of the electron locally is taken to be that which is appropriate to an electron with energy E. This approximation is valid as long as the potential varies sufficiently slowly so as not to change the character of the wavefunction. This approximation is very closely related to the WKB approximation but differs in that Bloch states are used as a basis for the approximation instead of plane waves. Thus the wavefunctions are of the form

*Recent calculations by Feuchtwang[18] indicate that when a more rigorous approach to the problem is taken the results are essentially of the same form.

$$\psi_{E,n,k_{\sim\|}}(x_{\sim}) = (k_{x,n}(E-\varphi(x))^{-\frac{1}{2}} U_{k,n}(x_{\sim}) e^{ik_{\sim\|}\cdot x_{\sim\|}}$$

$$\exp\left[i \int_{o}^{x} k_{x,n}(k_{\sim\|}, E-\varphi(x'))dx' \right] \qquad \text{(II-8)}$$

where we have assumed that $U_{k,n}(x)$ does not vary widely with k.

The computation of T(a,b) can be divided into four parts:

1) The wavefunction for state a in metal 1 is matched onto a state in the insulator with the same energy as state a at the interface between metal 1 and the insulator.

2) The wavefunction in the insulator is required to vary according to Schrödinger's equation until the second interface between the metal 2 and the insulator is reached.

3) The wavefunction at the insulator metal interface is matched onto state b in metal 2.

4) Finally, T(a,b) is computed from

$$T(a,b) = \frac{\int dydz \left|\psi_b(x=t)\right|^2}{\int dydz \left|\psi_a(x=o)\right|^2} \qquad \text{(II-9)}$$

Proceeding with this recipe we take the states at the interface between metal 1 and the insulator to be

$$\psi_a = e^{ik_{\sim\|}\cdot x_{\sim\|} ik_{xa}x} + Re^{ik_{\sim\|a}\cdot x_{\sim\|} -ik_{xa}x} \qquad \text{(II-10)}$$

$$\psi_T = \sum_n T_n (k_{xi,n}(x))^{-\frac{1}{2}} U_{\underset{\sim}{k},n}(\underset{\sim}{x}) e^{i\underset{\sim}{k}_{\parallel} \cdot \underset{\sim}{x}_{\parallel}} \exp\left[i \int_o^x k_{xi,n}(\underset{\sim}{k}_{\parallel}, E-\varphi(x'))dx' \right] \tag{II-11}$$

where ψ_a is the wavefunction of the electron in metal 1 and ψ_T is the wavefunction of the electron transmitted into the insulator. In Eq. II-11 we take the positive imaginary part of $k_{xi,n}$. Thus, we are neglecting multiple reflections. This approximation is excellent due to the large attentuation of the amplitude of the wave reflected at the second interface.

Assuming that the lattice is cleaved parallel to a plane of the crystal with rational indices, a set of lattice vectors can be chosen such that two of the vectors of the reciprocal lattice are contained in the cleavage plane. Let $\{\underset{\sim}{g}_p\}$ be the lattice vectors spanning the two dimensional lattice defined by the reciprocal lattice vectors in the plane parallel to the cleavage plane. The periodicity of $U_{\underset{\sim}{k},n}(\underset{\sim}{x})$ in y, and z implies that

$$U_{\underset{\sim}{k},n}(x=o,\underset{\sim}{x}_{\parallel}) = \sum_q A_{n,q} e^{i\underset{\sim}{g}_q \cdot \underset{\sim}{x}_{\parallel}} \tag{II-12}$$

$$\frac{\partial U_{\underset{\sim}{k},n}(x=o,\underset{\sim}{x}_{\parallel})}{\partial x} = \sum_r B_{n,r} e^{i\underset{\sim}{g}_r \cdot \underset{\sim}{x}_{\parallel}} \tag{II-13}$$

where $A_{n,q}$ and $B_{n,r}$ are in principle coefficients which can be calculated. The sums in Eqs. II-12 and II-13 run over all the two dimensional reciprocal lattice vectors. Applying the boundary conditions

$$\psi(x=0^-) = \psi(x=0^+)$$
$$\frac{\partial\psi}{\partial x}(x=0^-) = \frac{\partial\psi}{\partial x}(x=0^+) \qquad \text{(II-14)}$$

we obtain two results. First, the planar nature of the interface implies that

$$\underset{\sim}{k}_{\|a} = \underset{\sim}{k}_{\|i} + \underset{\sim}{g}_p \qquad \text{(II-15)}$$

where $\underset{\sim}{g}_p$ is the reciprocal lattice vector of the two dimensional lattice which brings $\underset{\sim}{k}_{\|a}$ into the first Brillouin zone of the lattice. Second, we obtain an expression for T_n, the amplitude for the electron in state a to enter the state denoted by n,

$$T_n = 2ik_{xa}(G^{-1})_{p,n}(k_{xi,n}(o))^{\frac{1}{2}} \qquad \text{(II-16)}$$

where

$$G_{n,p} = i(k_{xa}+k_{xi,n}(o))A_{n,p}+B_{n,p}$$

is the matrix which results from the matching. In Eq. II-16 the index p is that which denotes the reciprocal lattice vector used in II-15.

The variation of the factor $(k_{xi,n}(x))^{-\frac{1}{2}}$ with x in Eq. II-11 has been neglected. (Its variation with x must be small to make the semiclassical approximation appropriate.) This completes step 1 of the procedure outlined above.

The second step in the procedure is automatically satisfied since Eq. II-11 is an approximate solution to Schrödinger's equation. Application of similar techniques to steps 3 and 4 yields after some algebraic manipulation

$$V_2\int\frac{d^3k_a}{(2\pi)^3}\,\delta_{E_a,E_b}\,T(a,b) =$$

$$16k_{xa}^2\sum_r\sum_{n,n'}\frac{\left[k_{xi,n}(t)k_{xi,n}(o)k^*_{xi,n'}(t)k^*_{xi,n'}(o)\right]^{\frac{1}{2}}}{\left[i(k_{xi,n}(t)+k_{x_b})C_{n,r}-D_{n,r}\right]}$$

$$\frac{\exp\left[i\int_o^t(k_{xi,n}(E-\varphi(x'))-k_{xi,n}(E-\varphi(x'))dx'\right]}{\left[-i(k_{xi,n'}(t)+k_{x_b})C^*_{n',r}-D_{n',r}\right]} \qquad \text{(II-17)}$$

where the sum r runs over those indices defining reciprocal lattice vectors such that $\underset{\sim}{g}_r = \underset{\sim}{k}_{\parallel b} - \underset{\sim}{k}_{\parallel a} - \underset{\sim}{g}_p$, $E_a = E_b$, and for the given values of $\underset{\sim}{k}_{\parallel b}$ and E_b, k_{xb} is real. In Eq. II-17 $C_{n,r}$ and $D_{n,r}$ are coefficients (analogous to those appearing in II-12 and II-13) appearing in the expansions of $U_{\underset{\sim}{k},n}(\underline{x}_\parallel,t)$ and $\frac{\partial U_{\underset{\sim}{k},n}}{\partial x}(\underline{x}_\parallel,t)$.

Exact evaluation of Eq. II-17 is impossible, and would not be desirable if possible (see below). However, we expect the imaginary part of

$k_{xi,n}$ to vary widely with n. Thus, the terms in Eq. II-17 will be dominated by the term* for which the imaginary part of $k_{xi,n}$ is minimum. Due to the exponential dependence of the terms in Eq. II-17 on the imaginary part of $k_{xi,n}$, the sum in Eq. II-17 can be approximated to high accuracy by taking only the largest term in the sum. If we let ℓ denote the value of n for which the imaginary part of $k_{xi,n}$ is minimum, then Eq. II-17 reduces to

$$V_2 \int \frac{d^3k_b}{(2\pi)^3} \delta_{E_a,E_b} T(a,b) \approx$$

$$16k_{xa}^2 \left[\left| k_{xi,\ell}(t) \right|^2 \left| k_{xi,\ell}(o) \right|^2 \right]^{\frac{1}{2}} \left| (G^{-1})_{p,\ell} \right|^2 \qquad \text{(II-18)}$$

$$\sum_r \frac{1}{\left| \left[i(k_{xi,\ell}(t)+k_{xb})C_{\ell,r} - D_{\ell,r} \right] \right|^2} \exp\left[-2 \int_o^t \mathrm{Im} k_{xi,\ell}(x')dx' \right]$$

To simplify the notation the subscript ℓ and the Im indicating the imaginary part will not be indicated in the following calculations. Henceforth, k_{xi} will denote the imaginary part of $k_{xi,\ell}$.

In experiments performed so far on samples with metallic electrodes,** there is no indication that the pre-exponential factor in Eq. II-18 is

---

*It is improbable, but conceivable, that the term which dominates in Eq. II-17 is a function of energy. None of the presently available experimental data gives any indication of the presence of such an energy dependence.

**Variations in the pre-exponential factor have been observed in experiments on samples with semimetal electrodes at low temperatures (2°K). These variations result from the many band edges near the Fermi level of the semimetal.[19]

rapidly varying (affecting the shape of the I-V curve drastically) or significantly different from one (affecting the magnitude of the current). Consequently, we will take

$$V_2 \int \frac{d^3 k_b}{(2\pi)^3} \delta_{E_a, E_b} T(a,b) = e^{-2\int_o^t k_{xi}(x')dx'} \tag{II-19}$$

Substituting these results in Eq. II-14, we have

$$I_T(V) = \frac{2eA}{\hbar} \int dE_a \int \frac{d^2 k_{\parallel}}{(2\pi)^2} \exp\left[-2\int_o^t k_{xi}(\underset{\sim}{k}_{\parallel}, E-\varphi(x'))dx' \right] \tag{II-20}$$

$$(f_1(E_a) - f_2(E_a))$$

where we have restated all the functional dependence of k_{xi}. Eq. II-20 can be simplified slightly by defining

$$\xi(x) = E - \varphi(x) \tag{II-21}$$

Then Eq. II-20 becomes

$$I_T(V) = \frac{2eA}{h} \int dE_a \int \frac{d^2 k_{\parallel}}{(2\pi)^2} \exp\left[-2\int_{\xi(o)}^{\xi(t)} d\xi \, \frac{dx}{d\xi} \, k_{xi}(\underset{\sim}{k}_{\parallel}, \xi) \right] \tag{II-22}$$

$$(f_1(E_a) - f_2(E_a))$$

This is the equation which will be used to determine the E-k curve from

the current-voltage data for a given structure.

Many assumptions have been made in obtaining Eq. II-22. Consequently, it is important to see how these assumptions might affect the E-k curve determined in this manner. These assumptions can be divided into two groups. In this first group are those assumptions which change the nature of the pre-exponential factor in Eq. II-22. The nature of the states in the metals and the approximation of the factors in Eq. II-18 are included in this group. These assumptions will influence the determination of the E-k curve only when the true pre-exponential factors differ greatly in dependence on voltage and energy from the assumed dependence. Constant factors lead only to an offset in the E-k curve which can easily be removed by requiring the E-k curve to approach zero as E approaches the allowed bands of the insulator. Small differences in the energy dependence or bias dependence of the pre-exponential factors from the dependence above will lead to corrections in k_{xi} on the order of

$$\Delta k_{xi} \sim \frac{1}{2t} \log_e \delta(V,E) \qquad \text{(II-23)}$$

where $\delta(V,E)$ is the ratio of the assumed dependence to the correct dependence. For representative values of $t(= 30\ \text{Å})$ and $k_{xi}(= .33\ \text{Å}^{-1})$, $\delta(V,E) = 3$ produces only a 6% change in k_{xi}.

The second group of assumptions consists of those which affect the exponential factor itself. This group consists of: the use of the semi-classical approximation for the wavefunctions in the insulator, and the assumption of specular reflection at the interface. Both of these

assumptions must be considered carefully since as indicated above the exponential factor governs the behavior of the tunneling current. The semiclassical approximation is valid if the change in the magnitude of the "wavelength" (in this case it may be complex) per unit length is small compared to one, that

$$\left|\frac{d}{dx}\left(\frac{1}{|k_{xi}(x)|}\right)\right| < | \qquad \text{(II-24)}$$

or

$$\left|\frac{d}{dE}\left(\frac{1}{|k_{xi}(E)|}\right)\frac{d\varphi}{dx}\right| < | \qquad \text{(II-25)}$$

This condition is easily satisfied for most tunneling experiments. For example, for representative values of k_{xi} (= .3 Å^{-1}) and $\frac{dk_{xi}}{dE}$ (= .2 $\text{eV}^{-1}\text{-Å}^{-1}$), the inequality in Eq. II-25 is satisfied if $\frac{d\varphi}{dx} < .45$ eV -Å^{-1}. For a sample which is 30 Å thick this implies a total bias (built-in plus applied) of less than 14 volts. This condition is satisfied for the biases applied in most tunneling experiments. When $|k_{xi}|$ is small, inequality II-25 may not be satisfied rigorously. However the modification to the assumed form of the wavefunction due to the breakdown of the WKB approximation is predominantly in the pre-exponential factor.

The assumption of specular reflection at the interface links together the parallel component of the propagation vector across both of the interfaces. On the other hand, diffuse reflection would cause a mixing of the various parallel components of the propagation vector in going

across the interfaces and would result in a change in the pre-exponential factor by the addition of a function weighting the various $\underset{\sim}{k}_{\|}$. As noted above there is no evidence that any pre-exponential factor affects the current in a significant manner. Consequently, the question of diffuse or specular reflection at the barrier interface is really not settled by the measured I-V, and it does not form a serious obstacle in the determination of the E-k curve.

Thus, we see that in spite of all the assumptions necessary to derive Eq. II-22 it is very useful and accurate for obtaining E-k curves for insulators. However, the most convincing justification of Eq. II-22 is the fact that most of the dependences in Eq. II-22 have been verified experimentally.

III. DISCUSSION OF TECHNIQUE FOR SOLVING THE INTEGRAL EQUATION

To obtain the E-k curve, we must solve Eq. II-22, given I as a function of V. Before attempting a solution to Eq. II-22, it is necessary to know both the thickness of the insulator region and the shape of the external potential distribution as a function of applied voltage. These quantities must be determined from independent experiments. Thus, all of the parameters and functions in Eq. II-22 are known except for $k_{xi}(\underset{\sim}{k}_{\|},\xi)$.

One of the more successful techniques for solving integral equations of the form of Eq. II-22 is a method which is analogous to Newton's method for obtaining the roots of a nonlinear equation.[20]

This method consists of using the integral equation to correct an initial guess iteratively until the solution is obtained to the desired accuracy. In order to see how the correction is predicted from the integral equation, consider the functional $\mathcal{L}$ defined by

$$\mathcal{L}\left\{k_{xi}(\underset{\sim}{k}_{\|},\xi),\ I_{exp}(V)\right\} = I_{exp}(V)-I_T(V) \qquad \text{(III-1)}$$

where $I_{exp}(V)$ is the experimental value of the current and $I_T(V)$ is given by Eq. II-22. From Eq. III-1, it follows that the solution is attained when $\mathcal{L} \equiv 0$. Let

$$k^o_{xi}(\underset{\sim}{k}_{\|},\xi) = k^j_{xi}(\underset{\sim}{k}_{\|},\xi)+\delta k^j_{xi}(\underset{\sim}{k}_{\|},\xi) \qquad \text{(III-2)}$$

where $\delta k^j_{xi}(\underset{\sim}{k}_{\|},\xi)$ is the correction necessary to make the j^{th} corrected E-k curve, $k^j_{xi}(\underset{\sim}{k}_{\|},\xi)$, equal to the solution, $k^o_{xi}(\underset{\sim}{k}_{\|},\xi)$.

Now consider

$$\mathcal{L}\left\{k^{o}_{xi}(k_{\sim\|},\xi), I_{exp}(V)\right\} =$$

$$\mathcal{L}\left\{k^{j}_{xi}(k_{\sim\|},\xi) + \delta k^{j}_{xi}(k_{\sim\|},\xi), I_{exp}(V)\right\} = 0 \qquad \text{(III-3)}$$

Expanding Eq. III-2 in a Taylor's series, we find

$$\mathcal{L}\left\{k^{j}_{xi}(k_{\sim\|},\xi), I_{exp}(V)\right\} + \int d^2k_{\|}\, d\xi \frac{\delta\mathcal{L}}{\delta k_{xi}(k_{\sim\|},\xi)} \delta k^{j}_{xi}(k_{\sim\|},\xi) + \ldots = 0 \qquad \text{(III-4)}$$

where $\frac{\delta\mathcal{L}}{\delta k_{xi}(k_{\sim\|},\xi)}$ is the variational derivative of the functional, $\mathcal{L}$, with respect to the function $k_{xi}(k_{\sim\|},\xi)$ evaluated at

$$k_{xi}(k_{\sim\|},\xi) = k^{j}_{xi}(k_{\sim\|},\xi) \qquad \text{(III-5)}$$

Neglecting the higher order terms in Eq. III-4, we have a linear integral equation for the correction to $k^{j}_{xi}(k_{\sim\|},\xi)$,

$$\int d^2k_{\|}\, d\xi \frac{\delta\mathcal{L}}{\delta k_{xi}(k_{\sim\|},\xi)} \delta k^{j}_{xi}(k_{\sim\|},\xi) = -\mathcal{L}\left\{k_{xi}(k_{\sim\|},\xi), I_{exp}(V)\right\} \qquad \text{(III-6)}$$

or formally

$$\delta k^{j}_{xi}(k_{\sim\|},\xi) = -\int dV \left(\frac{\delta\mathcal{L}}{\delta k_{xi}(k_{\sim\|},\xi)}\right)^{-1} \mathcal{L}\left\{k_{xi}(k_{\sim\|},\xi), I_{exp}(V)\right\} \qquad \text{(III-7)}$$

where $\left(\frac{\delta\mathcal{L}}{\delta k_{xi}(k_{\sim\|},\xi)}\right)^{-1}$ is the inverse of the integral operator in equation III-6, and satisfies the relation

$$\int dV \left(\frac{\delta \mathcal{L}}{\delta k_{xi}(k_{\sim\|}^{1}, \xi^{1})} \right)^{-1} \frac{\delta \mathcal{L}}{\delta k_{xi}(k_{\sim\|}, \xi)} = \delta(\xi - \xi^{1}) \delta(k_{\sim\|} - k_{\sim\|}^{1}) \ .$$

Equation III-6 together with the procedure for obtaining the $j+1^{th}$ corrected value from the j^{th}, defined by the equation

$$k_{xi}^{j+1}(k_{\sim\|}, \xi) = k_{xi}^{j}(k_{\sim\|}, \xi) + \delta k_{xi}^{j}(k_{\sim\|}, \xi) \ , \qquad \text{(III-8)}$$

forms the basis of an iterative procedure which allows determination of $k_{xi}(k_{\sim\|}, \xi)$ to any accuracy desired.

IV. NUMERICAL SOLUTION

Before discussing in detail the numerical solution of Eq. II-22 using the technique outlined in section III, it is necessary to discuss in more detail some of the aspects of Eq. II-22. First, we will consider the form of the potential, $\varphi(x)$, in the insulator. Several factors, image force, space charge, and field penetration into the metal, can cause deviations in the form of the potential from the simple trapezoidal barrier. All of these effects have been shown to be small and can be neglected. The discussion given by Thornber, et al.[21] indicates that the static dielectric constant is appropriate in the discussion of image force effects upon the barrier shape in this type of tunneling process. The relatively large value of the static dielectric constant of insulators makes the correction to the barrier shape due to image forces negligible. The possibility of space charge changing the shape of the barrier can only be ruled out by careful experimental study of the insulator region. However, the relatively large density of charged centers ($N \sim 10^{19}$ 1/cm^3) required to change the potential by a significant amount ($\Delta\varphi \sim .1$eV) for the thicknesses encountered in tunneling samples ($t \sim 30$ Å) makes it improbable that enough space charge would exist in the insulator to produce significant changes in the barrier. Thus, we will neglect the influence of space charge upon the shape of the barrier. Field penetration into the metal modifies the barrier shape only over distances of a few Ångstroms near the metal electrode, and its effect is small.[22,23] Thus, it will be neglected. Consequently, we will take the barrier to be trapezoidal in shape as indicated in Fig. 2.[21]

The temperature dependence of the tunneling current in MIM

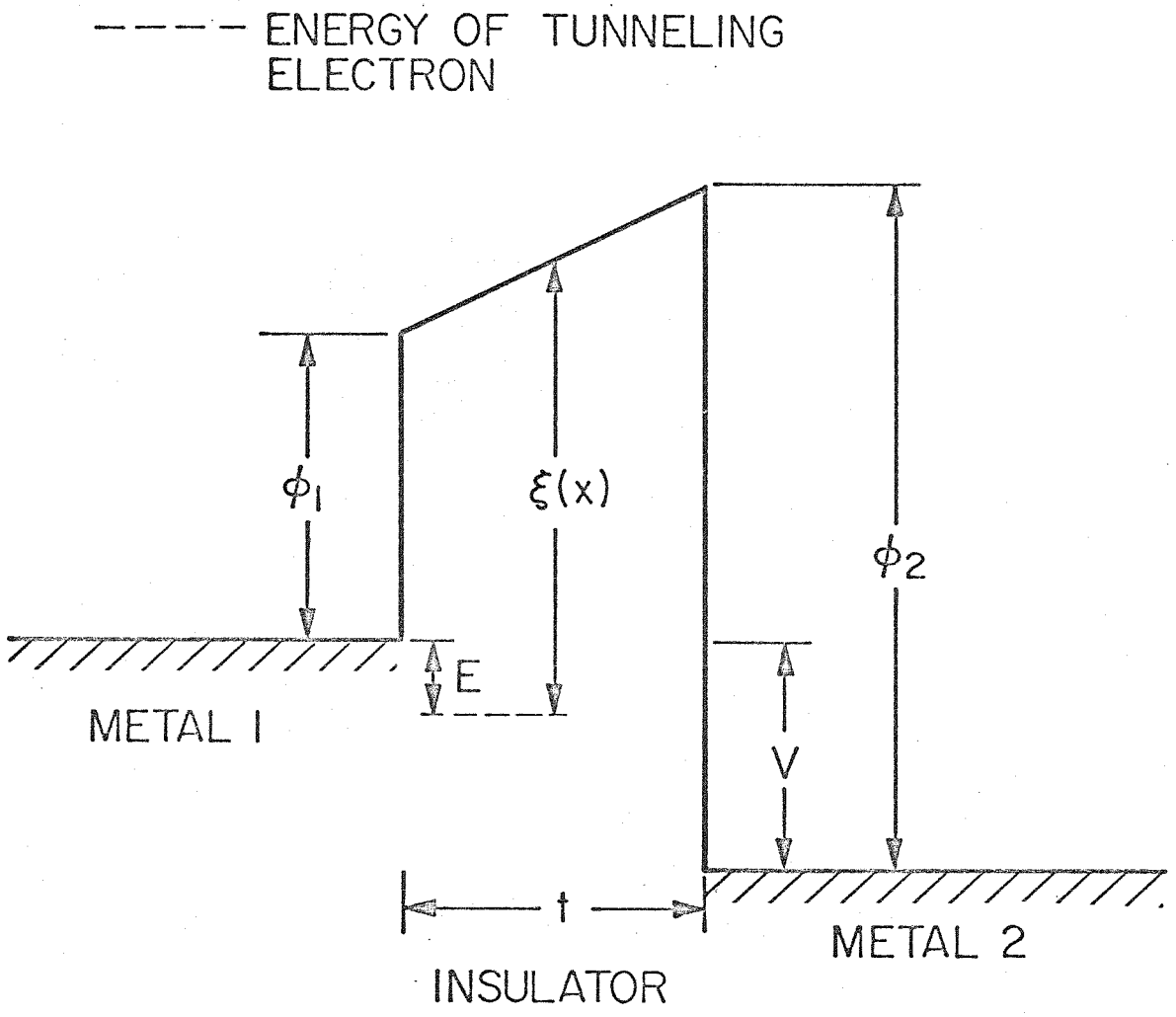

Figure 2. Schematic diagram of metal-insulator-metal structure with the various parameters in the expression for the tunneling current defined.

structures plus simple calculations of tunneling currents in MIM structures indicate that in all structures the temperature dependence of the current can be eliminated by going to sufficiently low temperatures. The temperature at which this condition is reached depends upon the E-k curve and the value of the applied voltage. However, for E-k curves similar to the one for AlN (discussed below) little error is made in applying the T=0 limit to the data taken at room temperature. Thus, we take T=0. This assumption can be relaxed with some difficulty in the numerical calculation; however, it is more convenient for the experiments to be performed at temperatures such that the approximation is valid.

As pointed out in section II, the tunneling current is dominated by the behavior of the exponential factor. This factor varies widely for small changes in k_{xi}. Consequently, it is possible to approximate the exponential factor about its maximum in $\underset{\sim}{k}_{\|}$ without imposing upon the E-k data any arbitrary constraint which is not already imposed by the limitations in the accuracy of the I-V data itself. In order to approximate the behavior of the integral in the exponent about its minimum as a function of $\underset{\sim}{k}_{\|}$, the dependence of $k_{xi}(\underset{\sim}{k}_{\|},\xi)$ on $\underset{\sim}{k}_{\|}$ about this minimum must be ascertained. Using the results of the analytic form which have been obtained in the calculation of Kane[9] as a guide, we take

$$k_{xi}^2(\underset{\sim}{k}_{\|},\xi) = g(\xi) + \alpha k_{\|}^2 \qquad \text{(IV-1)}$$

where $g(\xi)$ is an arbitrary function. α, a dimensionless constant in Eq. IV-1, allows us to take into account anisotropy between directions in the insulator parallel and perpendicular to the plane of the interface.

Using the above assumptions plus the definition of the various variables defined in Fig. 2, Eq. II-22 reduces to

$$I_T(V) = \frac{Ae\alpha}{t\hbar(2\pi)^2}\,(\varphi_2-\varphi_1-V)\int_o^V dE\,\exp\left[\frac{-2t}{(\varphi_2-\varphi_1-V)}\int_{\varphi_1+E}^{\varphi_2+E-V} k(\xi)d\xi\right] \qquad \text{(IV-2)}$$

where $k(\xi) = \sqrt{g(\xi)}$. In deriving Eq. IV-2, we have taken $V < \varphi_2$ and $V < E_g-\varphi_1$ where E_g is the energy gap of the insulator. This condition requires that the electrons tunnel through the constant thickness portion of the barrier only and not through the triangular part of the trapezoidal barrier. Of course, the current for higher voltages has information about the E-k curve in it. However, for these voltages the variation in the thickness over which some of the electrons tunnel masks the information about the E-k curve. Thus, it is desirable to attempt to sue the I-V data for $V > \varphi_2$, or $V > E_g-\varphi_1$ in obtaining the E-k curve.

Applying the technique outlined in section III, we have the set of equations corresponding to Eq. III-6 and III-8.

$$I_T(V)-I_{exp}(V) = \int_{a_1(V)}^{a_2(V)} G(V,\xi)\delta k(\xi)d\xi \qquad \text{(IV-4)}$$

and

$$k^{j+1}(\xi) = k^j(\xi) + \delta k^j(\xi) \qquad \text{(IV-4)}$$

to be iterated to obtain a solution for the E-k curve. $G(V,\xi)$ is defined in Table I where

$$\Gamma(\xi,V,E) = \frac{e}{\hbar(2\pi)^2} \alpha A \frac{L(V,E)}{F(V,E)} \left[\frac{1}{k^2(\xi)F(V,E)} \right]^{-2} \frac{t}{(\varphi_2 - \varphi_1 - V)} \qquad \text{(IV-5)}$$

and

$$L(V,E) = \exp\left[\frac{-2t}{(\varphi_2 - \varphi_1 - V)} \int_{\varphi_1+E}^{\varphi_2+E-V} d\xi' k(\xi') \right] \qquad \text{(IV-6)}$$

$$F(V,E) = \frac{t}{(\varphi_2 - \varphi_1 - V)} \int_{\varphi_1+E}^{\varphi_2+E-V} \frac{d\xi'}{k(\xi')} \qquad \text{(IV-7)}$$

The values of $a_1(V)$ and $a_2(V)$ are given in Table II.

A computer program was written to carry out the technique described above. This program is discussed in some detail in Appendix B.

Table I

Definition of $G(\xi,V)$

Case I: $\varphi_2 > \varphi_1$; $V < (\varphi_2 - \varphi_1)/2$

Limits on ξ	$G(\xi,V)$
$\varphi_1 < \xi < \varphi_1 + V$	$\int_0^{\xi-\varphi_1} dE\ \Gamma(\xi,V,E)$
$\varphi_1 + V < \xi < \varphi_2 - V$	$\int_0^{V} dE\ \Gamma(\xi,V,E)$
$\varphi_2 - V < \xi < \varphi_2$	$\int_{\xi-\varphi_2+V}^{V} dE\ \Gamma(\xi,V,E)$

Table I

Definition of $G(\xi,V)$

Case II: $\varphi_2 > \varphi_1$; $(\varphi_2-\varphi_1)/2 < V < \varphi_2-\varphi_1$

Limits on ξ	$G(\xi,V)$
$\varphi_1 < \xi < \varphi_1 + V$	$\int_0^{\xi-\varphi_1} dE\ \Gamma(\xi,V,E)$
$\varphi_2 - V < \xi < \varphi_1 + V$	$\int_{\xi-\varphi_2+V}^{\xi-\varphi_1} dE\ \Gamma(\xi,V,E)$
$\varphi_1 + V < \xi < \varphi_2$	$\int_{\xi-\varphi_2+V}^{V} dE\ \Gamma(\xi,V,E)$

Table I

Definition of $G(\xi,V)$

Case III: $\varphi_2 > \varphi_1$; $\varphi_2 - \varphi_1 < V < \varphi_2$

Limits on ξ	$G(\xi,V)$
$\varphi_2 - V < \xi < \varphi_1$	$-\int_{o}^{\xi-\varphi_2+V} dE\ \Gamma(\xi,V,E)$
$\varphi_1 < \xi < \varphi_2$	$-\int_{\xi-\varphi_1}^{\xi-\varphi_2+V} dE\ \Gamma(\xi,V,E)$
$\varphi_2 < \xi < \varphi_1 + V$	$-\int_{\xi-\varphi_1}^{V} dE\ \Gamma(\xi,V,E)$

Table I

Definition of $G(\xi,V)$

Case IV: $\varphi_1 > \varphi_2$

Limits on ξ	$G(\xi,V)$
$\varphi_2 - V < \xi < \varphi_2$	$-\int_0^{\xi-\varphi_2+V} dE\ \Gamma(\xi,V,E)$
$\varphi_2 < \xi < \varphi_1$	$-\int_0^{V} dE\ \Gamma(\xi,V,E)$
$\varphi_1 < \xi < \varphi_1 + V$	$-\int_{\xi-\varphi_1}^{V} dE\ \Gamma(\xi,V,E)$

Table II

Limits of Integration on Equation 26

Conditions	$a_1(V)$	$a_2(V)$
$\varphi_2 > \varphi_1$; $V < (\varphi_2 - \varphi_1)/2$	φ_1	φ_2
$\varphi_2 > \varphi_1$; $(\varphi_2 - \varphi_1)/2 < V < \varphi_2 - \varphi_1$	φ_1	φ_2
$\varphi_2 > \varphi_1$; $\varphi_2 - \varphi_1 < V < \varphi_2$	$\varphi_2 - V$	$\varphi_1 + V$
$\varphi_1 > \varphi_2$	$\varphi_2 - V$	$\varphi_1 + V$

V. CRITERIA FOR EXPERIMENTAL DATA

A number of electron transport mechanisms in addition to the tunneling mechanism described here might be responsible for the dependence of the current on voltage observed for a MIM structure with a thin insulating layer. Consequently, it is necessary to make a number of experimental checks to see if the simple tunneling model is applicable before any attempt is made to interpret the I-V characteristics in terms of the E-k relation for the insulating layer. While it is not possible to rule out experimentally all mechanisms for electron transport except the mechanism discussed here, it is possible to test a given set of experimental data with certain stringent criteria to check the applicability of the model. These criteria are:

1. All of the parameters entering into the model except for the E-k curve itself must be determined by experiments independent of the actual tunneling experiments.
2. I-V data should be available on tunneling samples with different thicknesses and different metal electrodes. The E-k relation determined from the I-V data on these different samples must agree (within some reasonable limit of error) in the energy range where the I-V data give a reliable determination of the E-k relation (see section VI).
3. The I-V characteristic should have been measured upon a sample with one of the metal electrodes in the supercon-

ducting state.* The superconducting gap of the metal electrode must be observed in this Giaever tunneling experiment.

Let us discuss briefly these various criteria. A wide enough variety of experiments can be performed on MIM structures to make it possible to satisfy criterion one. The area of the sample may be determined by measuring the dimension of the metal electrode using a microscope. The thickness of the insulating layer may be determined from the capacitance of the sample in conjunction with the measured area. Photoemission experiments[25] in which electrons are excited in the metal electrodes by monochromatic radiation and then traverse the insulating layer allows the determination of both the barrier energies, φ_1 and φ_2. The barrier energies may also be determined by studying the I-V characteristics of samples with insulating layers which are thick enough to make thermal excitation of electrons over the barrier the predominate mechanism for current transport through the insulator.[26] The degree to which the results of the photoemission studies and the studies of the thermal currents agree with those expected when the insulating layer is described by a trap free layer and the barrier is described by a trapezoidal shape barrier gives a measure of how accurately the model used here describes the insulating region. Large deviations[27] from the results expected should be examined carefully to determine what aspect of the model is causing the deviation and what effect the variation in this aspect from the assumed model might have upon the tunneling current.

Criterion two provides a very strong check on the model itself. If

*The author is grateful to C. B. Duke for pointing out this test in his unpublished manuscript.[24]

the E-k curve is independent of the thickness of the insulator, then we have experimentally verified that the equation for the tunneling current has the correct dependence on the thickness of the insulator. It is improbable that any mechanism for current transport through the insulator other than tunneling would have this precise thickness dependence. In addition, the variation of barrier potential (φ_1 and φ_2) with the metal electrode allows us to verify experimentally the energy dependence in the equation for the tunneling current without changing the applied bias. If the experimental data satisfy this requirement, then the two major dependences in the model have been experimentally verified.

In addition to these important checks on the applicability of the model provided by this criterion, it eliminates the possibility of several errors which may seriously affect the accuracy of the results. The accuracy of the E-k curve is directly proportional to the accuracy of the determination of the thickness of the insulator. Thus, close agreement between the E-k relation obtained for samples with different thicknesses implies that the determination of the thickness of the sample by using its capacitance is accurate.

The variation of the E-k curve from sample to sample puts an upper bound upon the fluctuations in the thickness of the insulator over the area of the sample. To illustrate this point and to demonstrate how the criterion under discussion eliminates the possibility of this type of error, consider the following model: Let the structure consist of various areas A_i with insulator thickness t_i. The capacitance of this structure is given by

$$C = \epsilon \sum_i \frac{A_i}{t_i} \tag{V-1}$$

or

$$C = \epsilon A \left\langle \frac{1}{t} \right\rangle$$

where A is the total area and

$$\left\langle \frac{1}{t} \right\rangle = \frac{1}{A} \sum_i A_i / t_i \tag{V-2}$$

Thus, the capacitance measures the average value of the inverse of the thickness. Now consider the tunneling current

$$I_T(V) = \sum_i A_i J(V, t_i) \tag{V-3}$$

where $J(V,t_i)$ is the current density for an applied voltage V and an insulator thickness t_i. It should be noted that $J(V,t_i)$ is exponentially dependent on t_i. Thus, its dependence on thickness is vastly different from the capacitance. If we attempt to force V-3 to be of the form

$$I_T(V) = AJ(V,t) \tag{V-4}$$

there will in general be no simple relationship between the t appropriate to Eq. V-4 and that obtained from Eq. V-2 unless all of the areas have

very nearly the same thickness. Thus, if large fluctuations in the thickness of the insulator existed across the sample area, the E-k curve could not be determined from the I-V data since the appropriate thickness would be undetermined. On the other hand, if the E-k for samples of appreciably different thickness is found to be the same when the thickness as measured by the capacitance of the sample is used in Eq. V-4, we can be assured that the thickness fluctuations are small.

The dependence of the E-k relation on the metal electrodes of the sample gives an excellent check on the combined importance of the metal electrode's band structure and the spatially varying part of the electron potential introduced by the metal in the insulator in determining the tunneling current. Both of these factors have been neglected in the derivation of Eq. II-2. Thus, only small variations in the E-k curve for various metal electrodes would indicate that these factors are indeed negligible.

The third criterion provided another verification that the mechanism of current transport through the insulator is tunneling. Successful application of this test rules out a large number of non-tunneling mechanisms. However, this test does not rule out tunneling mechanisms differing from the mechanism described here. Thus, criterion three does not replace criterion two, but compliments it.

Thus, using the above criteria, it is possible to determine whether or not the model used here is applicable to measured current-voltage data. If all of the above tests are satisfied, then it is highly improbable that the model is inappropriate.

VI. EXAMPLE

To illustrate the technique described above, and to demonstrate its usefulness in obtaining E-k curves from I-V data, we have applied this technique to the I-V data taken by Lewicki et al. on Al-AlN-(Mg,Au) MIM structures.[3,4] There are two reasons for selecting these data. First, the data form a well-documented case of tunneling through an insulator (most of the criteria of section V were checked); second, it is not valid to interpret the tunneling current through the Al-AlN-Au structures in terms of the standard approximate expressions[28] because of the large width in energy of the distribution of tunneling electrons. Consequently, interpretation of these data presents a worthwhile test of the technique discussed above.

Let us review briefly the relevant properties of AlN. Disordered AlN, used in the above mentioned structures, is an insulator with a 4.2 eV band gap. In disordered materials, α (see section IV) may be taken to be one by symmetry. Electron barrier energies of 1.53, 1.68, and 3.0 eV are formed at the interface between Mg, Al, and Au, (respectively), and AlN. A detailed description of the experimental structures and the various tests performed on the experimental data to test the validity of the tunneling model can be found in references 3 and 4.

The initial guess for the E-k relation used in the numerical, self-consistent analysis of the I-V curves for the AlN structures was taken to be the two band model,

$$k(E) = \left[\frac{2m_e m^*}{\hbar^2 E_g}(E_g - E)E\right]^{\frac{1}{2}} \qquad \text{(VI-1)}$$

where m_e is the mass of the electron, m^* is the effective mass of the material, Eg is the band gap and $\hbar$ is Dirac's constant. The values of m^* and Eg were taken to be .45, and 4.2 eV, respectively. These values are approximately those that Lewicki[3,4] found in his determination of the E-k curve for AlN for energies less than 1.8 eV.

First, consider the tunneling current through the Al-AlN-Mg structures. In Fig. 3, the experimental I-V for a 36.6 Å thick AlN layer is presented. Applying the self-consistent technique discussed above to these I-V data, we obtain the points on the $E\text{-}k^2$ relation (k^2 is plotted instead of k to make it possible to measure the effective mass near the valence and conduction band easily) represented by the circles in Fig. 4. For comparison we have also included the initial guess curve in Fig. 4. It is noted that the calculated points fall very close to the initial guess. This is merely an indication of how close Lewicki's values were and does not represent how close one must be to self-consistency before the technique works (see discussion of the Al-AlN-Au I-V data given below). To demonstrate how close to self-consistency the $E\text{-}k^2$ relation obtained in this manner is, we have plotted in Fig. 3 the I-V curve calculated from the points on the $E\text{-}k^2$ relation given in Fig. 4. The agreement is excellent.

To indicate the relative importance of the contribution to the tunneling current of electrons with various energies below the Fermi level of metal 1, we define D(E,V), the distribution in energy of the tunneling electrons as a function of applied bias V. As illustrated in Fig. 5, D(E,V) is the relative number of electrons per second tunneling through the insulator at a given energy, E, below the Fermi level of metal 1.

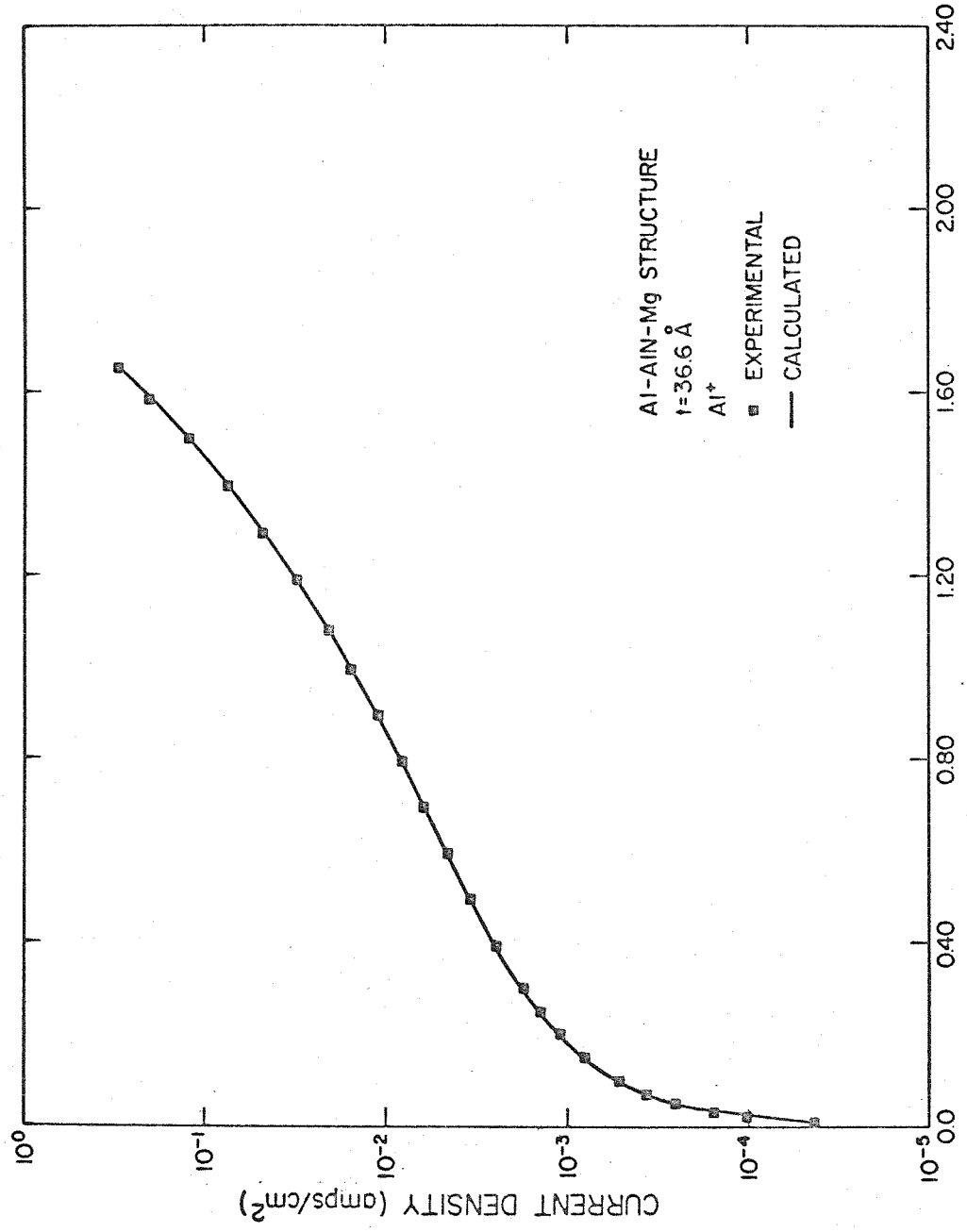

Figure 3. The experimental and calculated I-V curve for an Al-AlN-Mg structure.

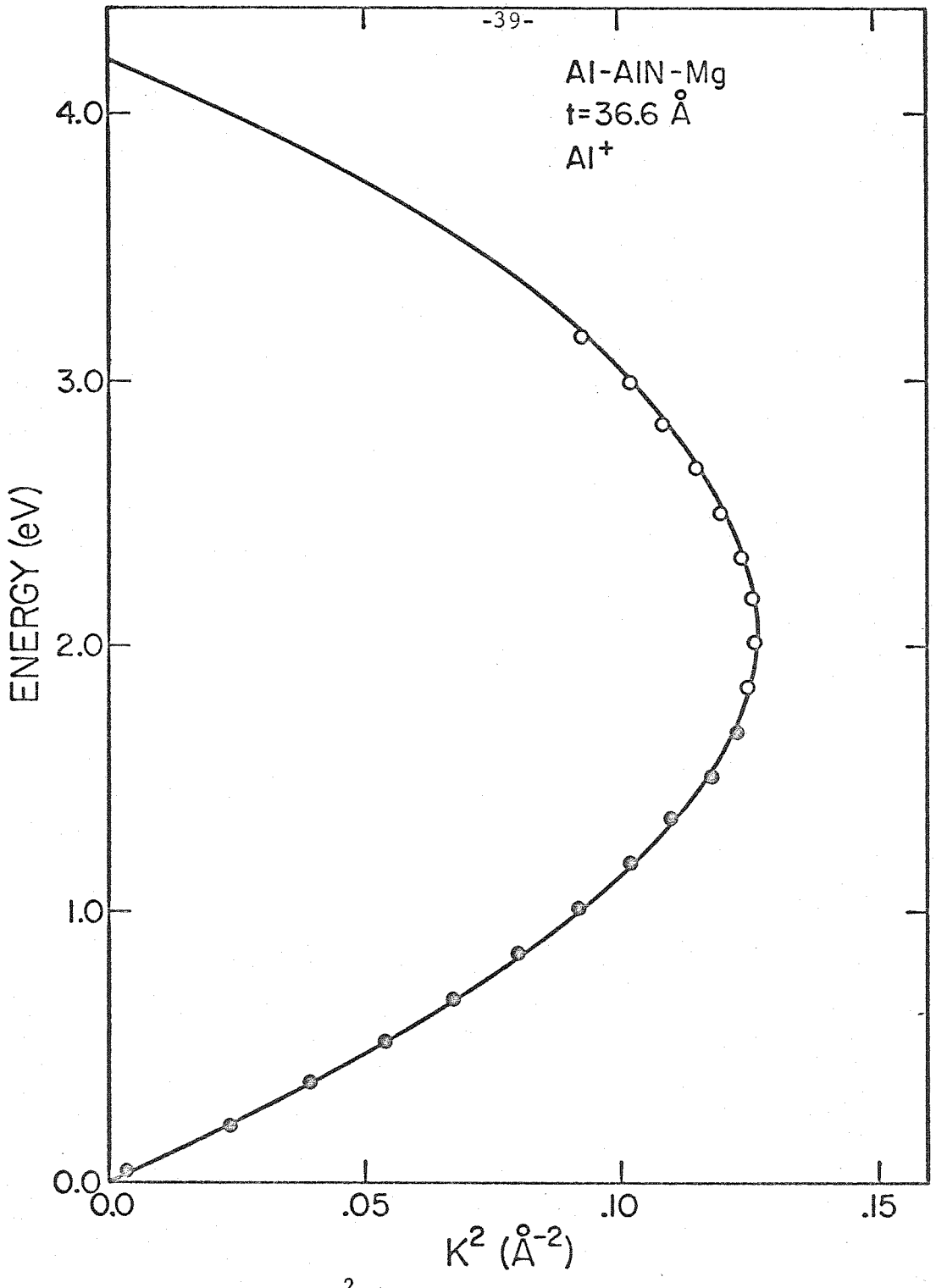

Figure 4. The E vs. k^2 curve for AlN obtained from the I-V data in Fig.3. The solid circles are relevant calculated points; the open circles are calculated points which should be disregarded (see text). The solid line is the E-k^2 curve for the two band model with $m^* = .45$, and $E_g = 4.2$ eV.

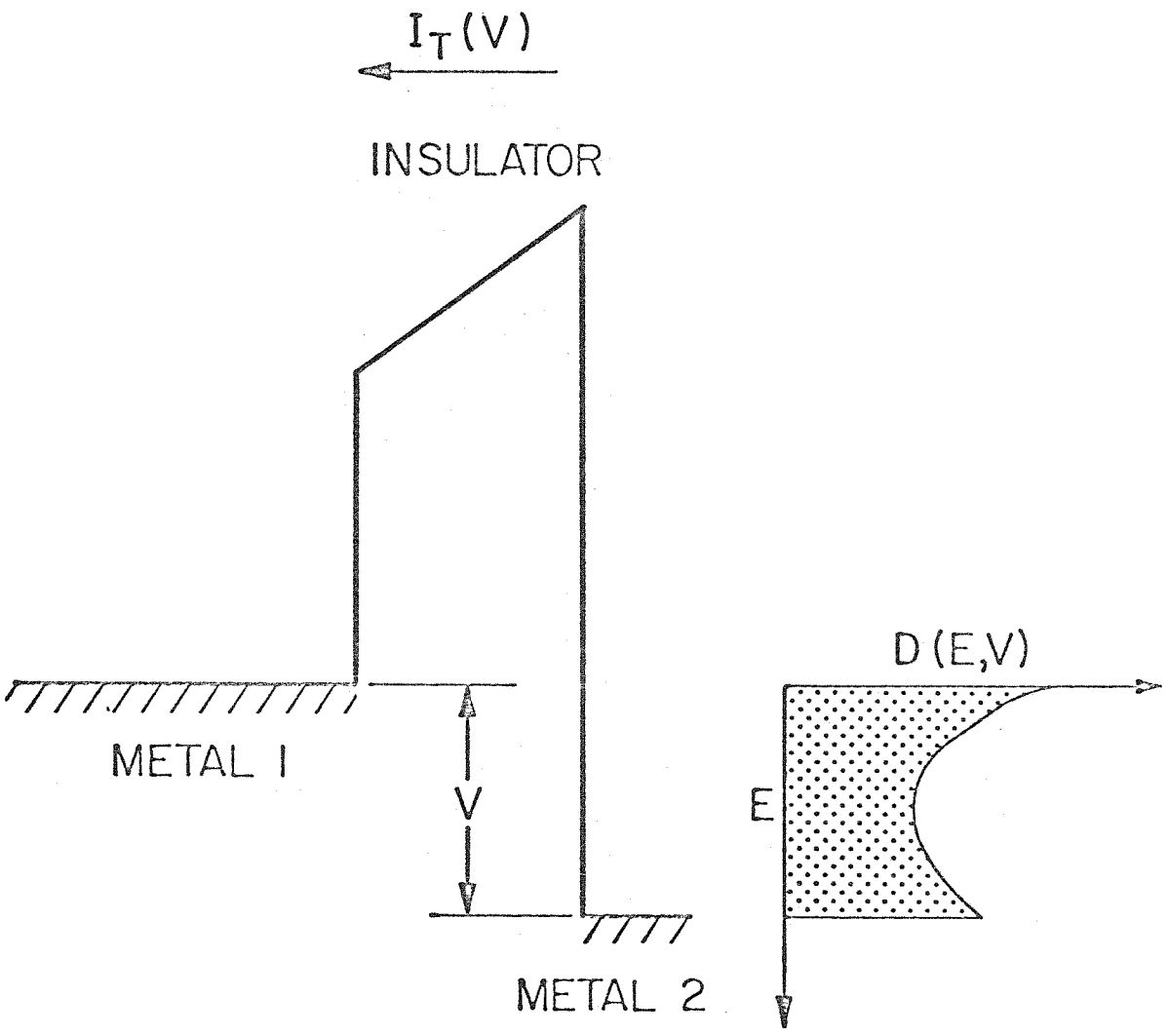

Figure 5. A schematic presentation of the definition of D(E,V).

Due to the zero temperature approximation, D(E,V) is non zero only for $0 \leq E \leq V$. These distributions are useful in studying two points. First, they indicate when the approximation schemes which assume that the distribution of tunneling electrons is sharply peaked about the Fermi level of metal 1 are appropriate. Second, they tell us what parts of the $E\text{-}k^2$ relation are determined accurately by the I-V data.

Let us consider this second point in more detail. The self-consistent method described here attempts to determine the $E\text{-}k^2$ relation for all the energies which are involved in the tunneling process from the complete I-V curve. However, the distribution of tunneling electrons maybe such that not all energies contribute a detectable fraction of the current for any voltage; consequently, that portion of the $E\text{-}k^2$ curve which is involved in the tunneling of electrons with these energies can not be obtained from the experimental data. Studying D(E,V) for various biases allows us to ascertain what portions of the E-k curve are accurately determined and what portions are merely remanents of the initial guess.

In Fig. 6 we show D(E,V) as a function of energy for three biases, 0.5, 1.0, and 1.6 volts. It should be noted that the current distributions are very sharply peaked about the Mg Fermi level in all three cases. Eighty per cent of the current is carried by electrons whose energies are within 0.4 of an eV of the Mg Fermi level. Thus, approximate methods for obtaining the E-k which assume that the distribution of the tunneling electrons is very sharply peaked about the Fermi level of the metal are appropriate in this case.

Careful study of the distributions of tunneling electrons shows

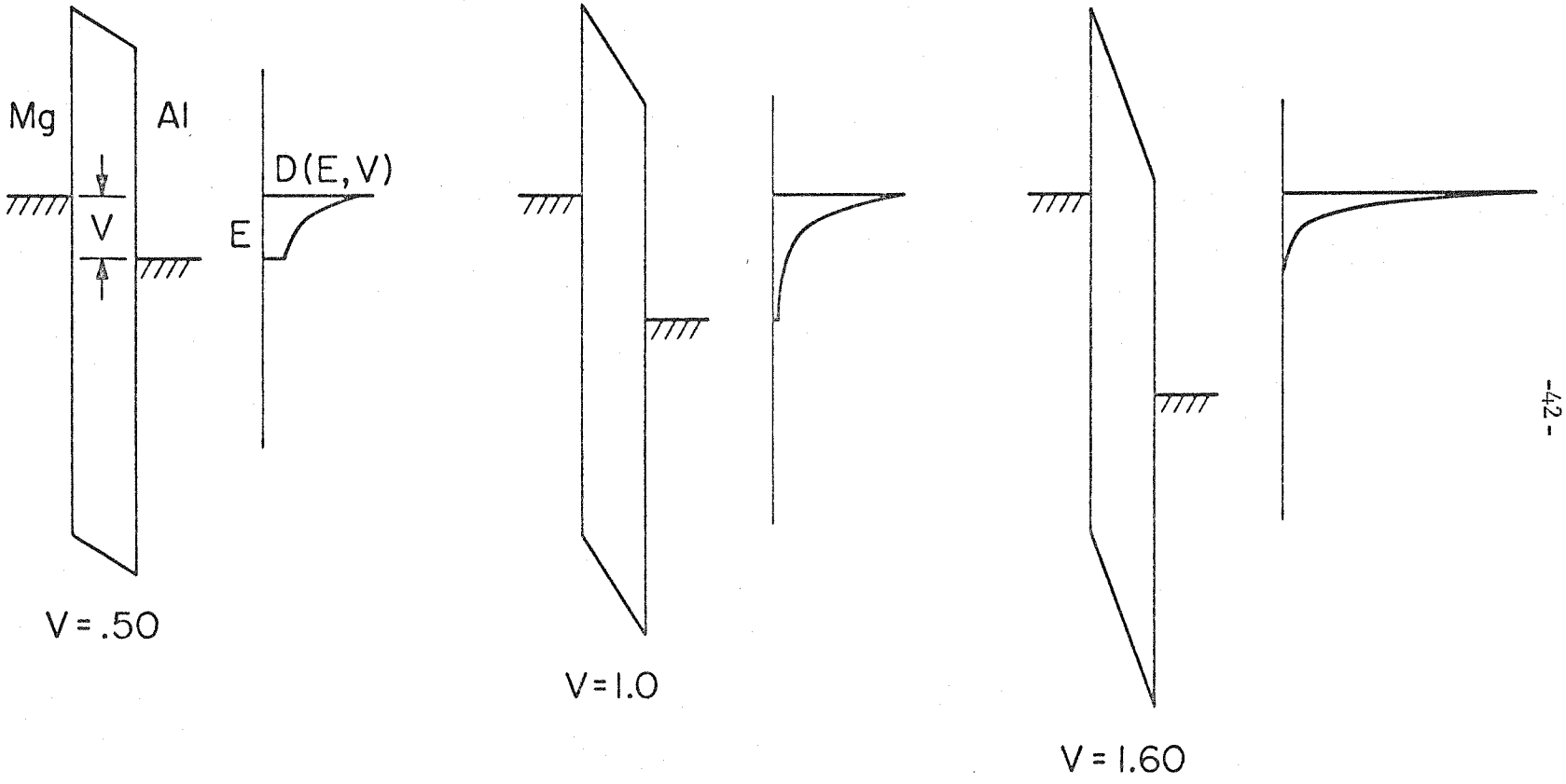

Figure 6. The distribution of tunneling electrons as a function of energy and applied bias for an Al-AlN-Mg structures.

that the portion of the E-k relation for energies greater than 1.8 eV does not contribute significantly to the determination of the I-V characteristic. Consequently, we expect the calculated points for energies greater than 1.8 eV to be very inaccurate. In fact in this calculation, they remain almost precisely at their initial value. To insure that these values of the E-k curve do not affect the determination of the $E\text{-}k^2$ relation for energies less than 1.8 eV, the self-consistent analysis was carried out using values from the solid curve in Fig. 10 as the initial guess values of the $E\text{-}k^2$ relation. The self-consistent analysis yielded values of the $E\text{-}k^2$ relation for energies less than 1.8 eV which were identical with those previously obtained, and for energies greater than 1.8 eV which were identical with the initial guess. Thus, we can disregard the points on the $E\text{-}k^2$ curve for energies greater than 1.8 eV.

Now consider the Al-AlN-Au structure. In Fig. 7, the I-V curve for a 30 Å Al-AlN-Au structure with the Au^+ is shown. In this case the I-V curve is ohmic for biases less than one volt. Furthermore, the large barrier height of Au on AlN allows the possibility of significant contributions to the tunneling current by electrons tunneling with energies just above the Fermi level of metal 2 (Au). These two points lead us to expect distributions of tunneling electrons with large energy widths. Thus, the approximate techniques are not applicable. This is a very serious limitation since the wide distributions imply that the I-V characteristic contains information about the $E\text{-}k^2$ relation for energies all the way to the valence band of AlN. However, the self-consistent technique discussed here allows the interpretation of these data. In Fig. 8 we present the points on the $E\text{-}k^2$ curve obtained from a self-consistent

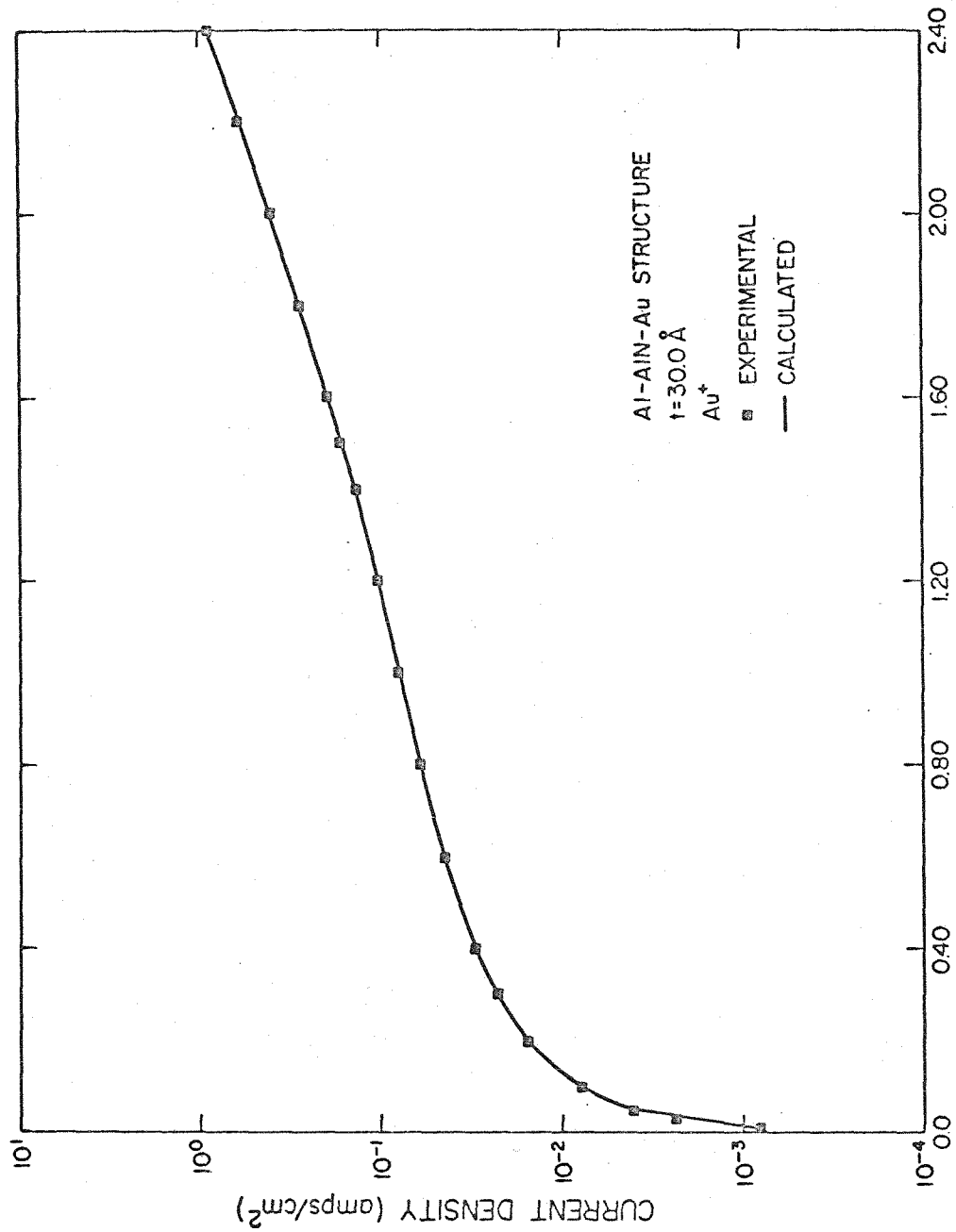

Figure 7. The experimental and calculated I-V curve for an Al-AlN-Au structure.

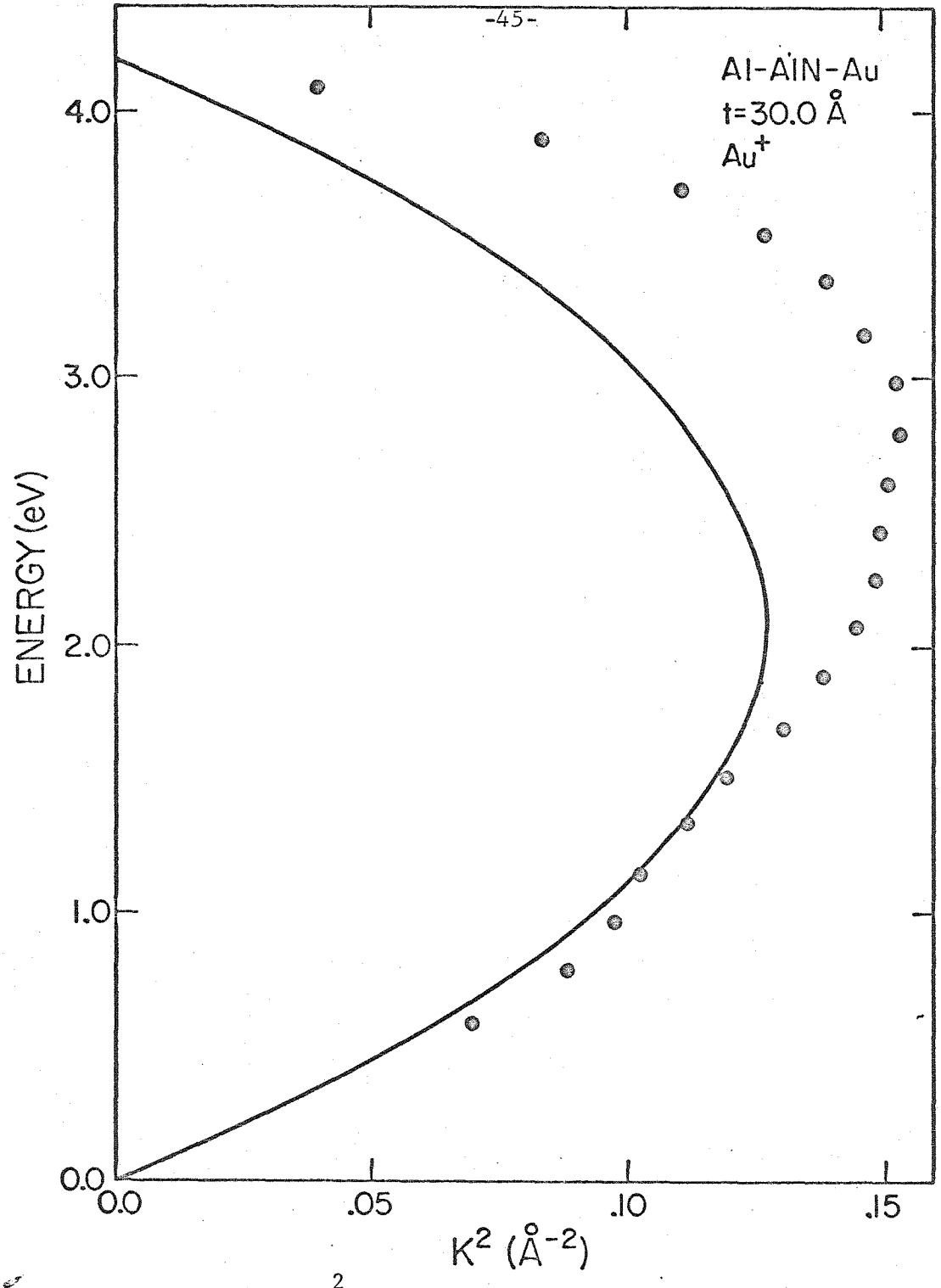

Figure 8. The E vs. k^2 curve for AlN obtained from the I-V data shown in Fig. 7. The solid circles are calculated points. The solid line is E-k^2 curve for the two band model with m* = .45 and E_g = 4.2.

analysis of the I-V data. For comparison we have again presented the curve used as the initial guess. The degree of self-consistency between the experimental I-V points and the I-V curve calculated using the points on the $E\text{-}k^2$ curve shown in Fig. 8 is shown in Fig. 7. Again the agreement is excellent.

In Fig. 9 we exhibit D(E,V) for the Al-AlN-Au structure for three different biases. The qualitative difference in the nature of the distributions of the tunneling electrons is evident on comparing Figs. 6 and 9. In the Au structures much of the tunneling current is carried by electrons with energies far from the Al Fermi level. In fact, for 2.40 volts applied bias, a significant fraction of the current is carried by electrons tunneling with energies slightly above the Fermi level of the Au. These very wide current distributions lead to the ohmic behavior of the Au structure for biases less than one volt, and the breakdown of any approximation scheme based upon expansions about the Fermi level.

In this case the $E\text{-}k^2$ relation is determined accurately all the way to the valence band. The points on the $E\text{-}k^2$ relation for energies greater than 1.8 eV differ significantly from their initial guess values. The values are significant in determining the I-V characteristic of the Al-AlN-Au structure; consequently, they cannot be disregarded.

In Fig. 10 we present the composite $E\text{-}k^2$ relation for AlN formed by combining the accurate points in Figs. 4 and 8. For comparison we have plotted also the points on the $E\text{-}k^2$ curve for AlN obtained by Lewicki et al.[3,4] from his analysis of the I-V data on Al-AlN-Mg structures. The agreement between all sets of values in excellent. At the present time no detailed theories of the electronic spectrum of disordered materials

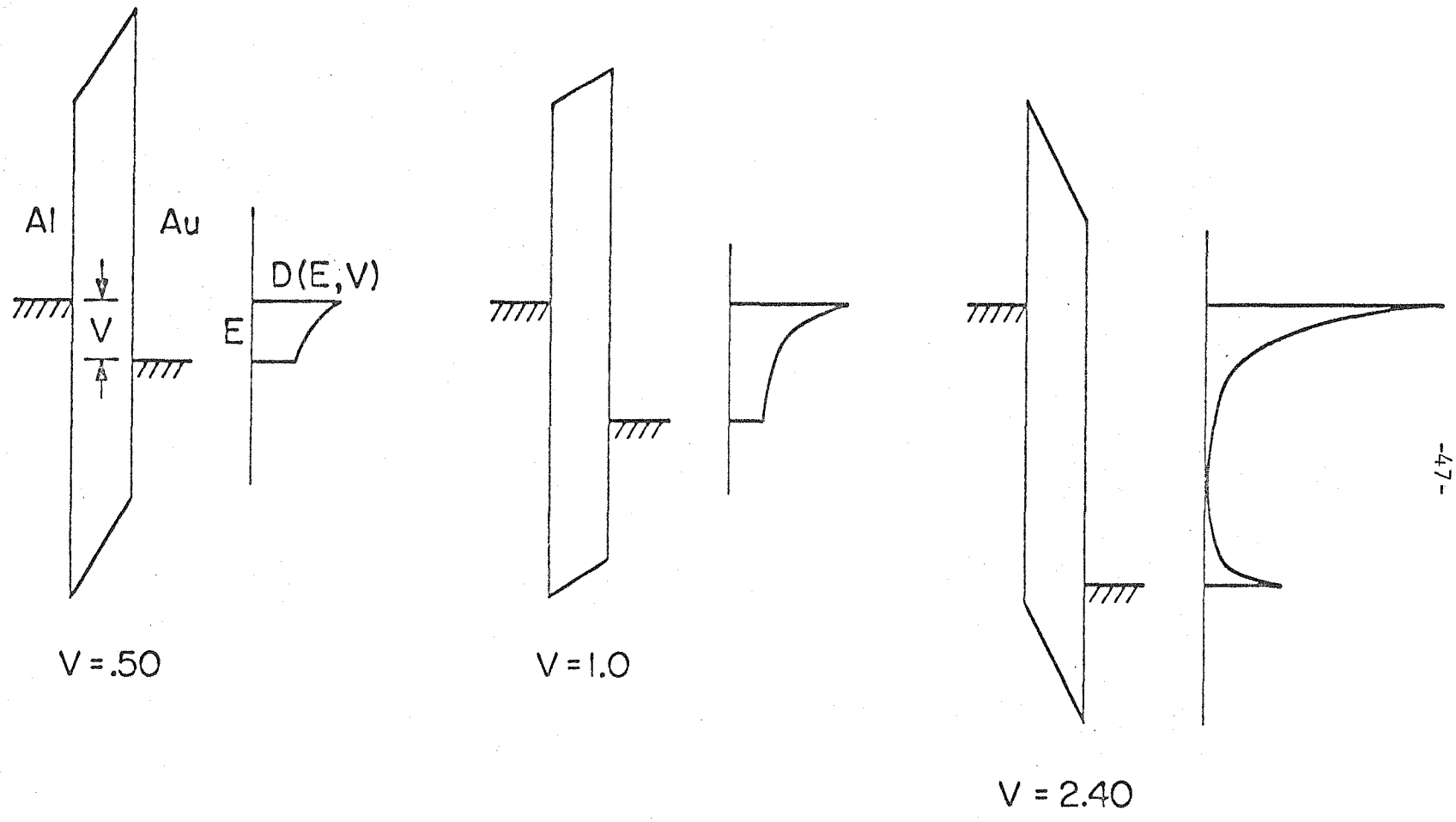

Figure 9. The distribution of tunneling electrons as a function of energy and applied bias for an Al-AlN-Au structure.

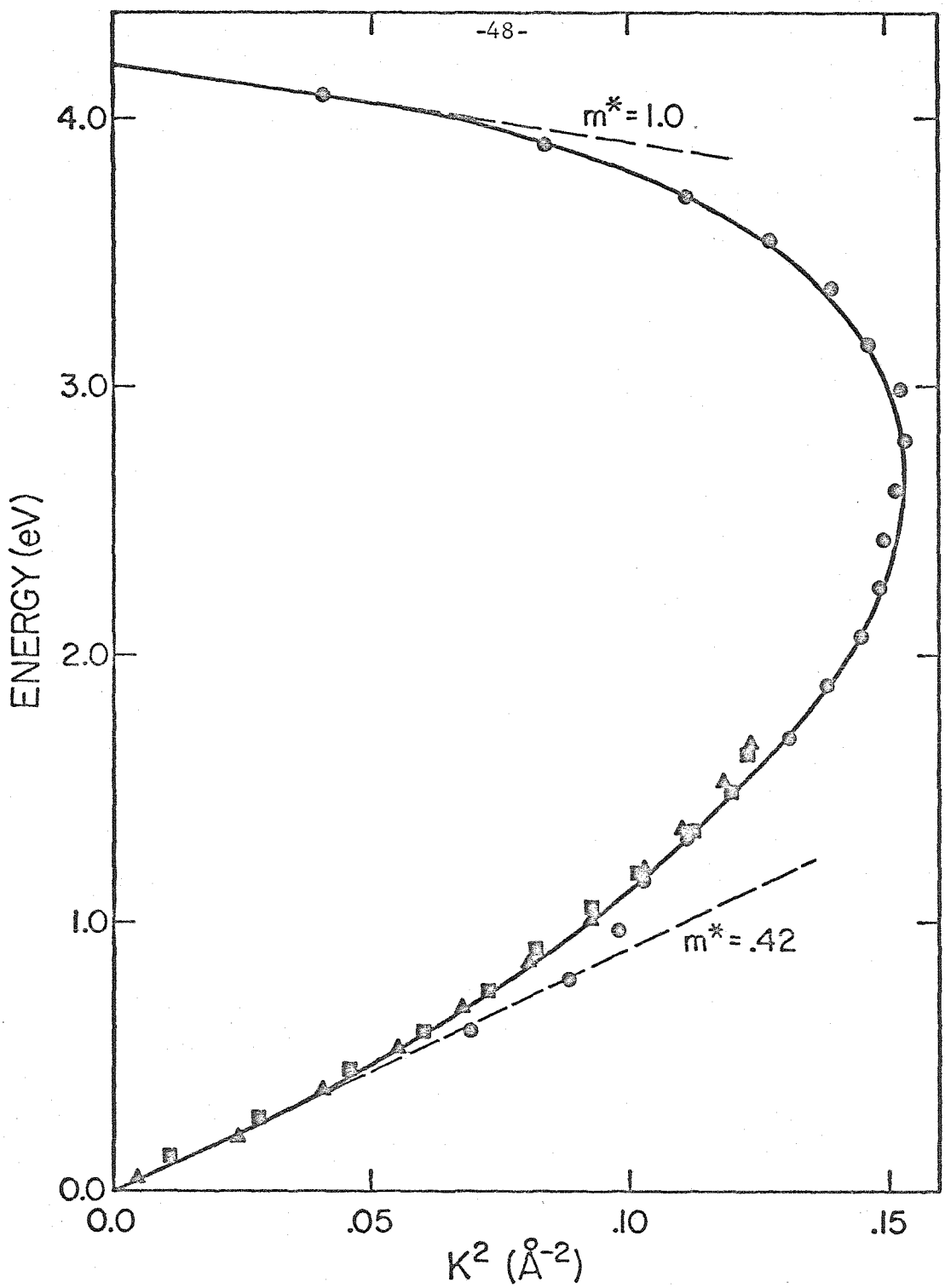

Figure 10. The composite E vs. k^2 curve for AlN. The triangles are the results of the analysis of the Al-AlN-Mg I-V data. The circles are the results of the analysis of the Al-AlN-Au I-V data. The squares are the results of Lewicki et al.'s analysis of the Al-AlN-Mg I-V data. The solid line is a smooth curve through the points.

exist. Thus, it is impossible to give a detailed discussion of the $E\text{-}k^2$ curve shown in Fig. 10. However, the $E\text{-}k^2$ curve is consistent with a picture of AlN having a rather broad conduction band with an effective mass of .42 and a very narrow valence band with an effective mass of approximately one. On comparing the initial guesses in Figs. 4 and 8 with the composite $E\text{-}k^2$ curve in Fig. 10, we conclude that the composite $E\text{-}k^2$ curve cannot be represented by any two band model (see Eq. VI-1) with a single effective mass and an energy gap of 4.2 eV. This points out even more clearly the necessity of not assuming any specific form for the E-k curve when attempting a general discussion of the tunneling.

VII. CONCLUSION

In this thesis we have examined carefully the basis for interpreting the I-V data on thin (thickness < 100 Å) insulator MIM structures in terms of a E-k curve for the insulator. The equation used to link the I-V data to the E-k relation was derived in a semi-rigorous manner making use of a simplified standard model. However, as indicated at the end of section II, the exact form of the final equation is unimportant as long as the exponential dependence of the tunneling current on the integral of the imaginary part of the propagation vector in the insulator is preserved. Because of the rather shaky theoretical position of the equation relating the I-V curve to the E-k curve, we presented in section V a detailed set of criteria for determining if a given set of I-V data is interpretable in terms of this model. It was found that if the experimental data satisfied these criteria, then the important dependences of the model on the thickness of the insulator and the energy of the tunneling electron is verified experimentally. However, the satisfying of these criteria does not completely rule out the possibility that the model is inappropriate. But it makes it improbable.

In section III and IV we presented a detailed numerical technique for obtaining the E-k curve for experimental I-V data regardless of the form of the distribution of the tunneling electrons producing the current. Section VI presents the results of the application of this technique to the data taken by Lewicki et al.[3,4] on AlN. The technique is found to be exceedingly successful. It allowed the determination of the E-k curve throughout the forbidden gap of the AlN, which cannot be accomplished by any of the approximate techniques.

APPENDIX A. DERIVATION OF THE EQUATION IV-3

By definition (Eq. III-1)

$$\mathcal{L}\left\{k(\xi), I_{exp}(V)\right\} = I_{exp}(V) - I_T(V) \tag{A-1}$$

where $I_T(V)$ is given by Eq. IV-2. Let us consider $\frac{\delta \mathcal{L}}{\delta k(\xi)}$. The most straightforward way of computing this variational derivative is to let

$$k(\xi) \rightarrow k(\xi) + \delta k(\xi) \tag{A-2}$$

then linearize the resulting expression in $\delta k(\xi)$. Then we note that the linear term in $\delta k(\xi)$ is of the form

$$\int \frac{\delta \mathcal{L}}{\delta k(\xi)} \delta k(\xi) d\xi \tag{A-3}$$

Performing this procedure on Eq. A-1, we obtain

$$\int \frac{\delta \mathcal{L}}{\delta k(\xi)} \delta k(\xi) d\xi = \int_o^V dE \int_{\varphi_1+E}^{\varphi_2+E-V} \Gamma(\xi, V, E) \delta K(\xi) d\xi \tag{A-4}$$

Interchanging the order of the integration gives the results indicated by Eq. IV-3 and Table I and II.

APPENDIX B. COMPUTER PROGRAM

The main purpose of the computer program described in this appendix is to make the computations necessary to solve Eqs. IV-3 and IV-4, iteratively. All of the computations except the solution of the integral equation involve straightforward computer programming. Consequently, we shall only discuss in some detail the solution of the integral Eq. IV-4 and leave to the listing of the program the answering of any questions of a more detailed nature.

To solve an integral equation of the form

$$\Delta I(V) = I_{exp}(V) - I_T(V) = \int_{a_1(V)}^{a_2(V)} G(V,\xi)\delta k(\xi)d\xi \qquad \text{(B-1)}$$

numerically, we must replace it by a finite set of linear equations. This is accomplished by approximating the integral on the right hand side of Eq. B-1 by one of the approximate integral techniques (Simpson's rule, Gaussian integration, etc.). In our case, Simpson's rule was most appropriate. Thus, Eq. B-1 can be approximated by

$$\Delta I(V_j) = \sum_{i=1}^{N} \tilde{G}(V_j,\xi_i)\delta k(\xi_i) \qquad \text{(B-2)}$$

where V_j is the value of the voltage at the N mesh points, ξ_i is the value of ξ at the N mesh points; and

$$\tilde{G}(V_j,\xi_i) = \Delta\xi C_i G(V_j,\xi_i) \qquad \text{(B-3)}$$

where $\Delta\xi$ is the mesh size in ξ and C_i is the appropriate constant for

Simpson's rule. Rewriting B-2 in matrix notation, we have

$$\tilde{G}\underset{\sim}{\delta k} = \underset{\sim}{\Delta I} \tag{B-4}$$

where $\underset{\sim}{\delta k}$ is the column vector of $\delta k(\xi_i)$, $\underset{\sim}{\Delta I}$ is the column vector of $\Delta I(V_j)$ and $\tilde{G}$ is the matrix of $G(V_j,\xi_i)$. Unfortunately, the solution of Eq. B-3 is an ill-posed problem (a small change in $\underset{\sim}{\Delta I}$ produces a rather large change in $\underset{\sim}{\delta k}$); and the direct matrix inversion leads to rapidly oscillating corrections, $\underset{\sim}{\delta k}$. Thus, it was necessary to stabilize Eq. B-3 by applying statistical techniques recently developed by J. N. Franklin.*[29] Basically, this technique consists of the following: Due to the finite number of places of accuracy in the numerical calculation and the fact that we are dealing with experimental data which have some error, the exact value of $\underset{\sim}{\Delta I}$ which should be substituted in Eq. B-4 is unknown. Thus we assume that

$$\underset{\sim}{\Delta I}_c = \underset{\sim}{\Delta I}_{exact} + \underset{\sim}{n} \tag{B-5}$$

where $\underset{\sim}{\Delta I}_{exact}$ is the value which should be substituted in Eq. B-4, and $\underset{\sim}{\Delta I}_c$ is the computed value. $\underset{\sim}{n}$ is a stochastic variable representing the uncertainties mentioned above. Making this substitution in Eq. B-4, we have

$$\tilde{G}\underset{\sim}{\delta k} + \underset{\sim}{n} = \underset{\sim}{\Delta I}_c \tag{B-6}$$

*The treatment given here is simplified and less general than that given by Franklin in reference 29.

where $\tilde{G}$ and $\Delta\underset{\sim}{I}_c$ are known, $\delta\underset{\sim}{k}$ and $\underset{\sim}{n}$ are unknown. Of course, Eq. B-6 cannot be solved for $\delta\underset{\sim}{k}$ given its statistical properties and the statistical properties of $\underset{\sim}{n}$.* Following Franklin we take

$$\delta\underset{\sim}{k}_s = L\Delta\underset{\sim}{I}_c \tag{B-7}$$

where L is a linear operator, and $\delta\underset{\sim}{k}_s$ is an estimate of the value of $\delta\underset{\sim}{k}$. One way of estimating $\delta\underset{\sim}{k}$ is to attempt to minimize the effect of $\underset{\sim}{n}$. Thus, we determine L from the condition

$$E\left\{\left|\underset{\sim}{e}\cdot(\delta\underset{\sim}{k}-L\Delta\underset{\sim}{I}_c)\right|^2\right\} = \text{minimum} \tag{B-8}$$

In Eq. B-8 $\underset{\sim}{e}$ is some vector in the space of $\delta\underset{\sim}{k}$ and E denotes the expectation value over the probability distribution for the above-mentioned stochastic variable. After some algebraic manipulations, we find that

$$L = (R_{\delta\underset{\sim}{k}\delta\underset{\sim}{k}}\tilde{G}^T)(\tilde{G}R_{\delta\underset{\sim}{k}\delta\underset{\sim}{k}}\tilde{G}^T+R_{\underset{\sim}{n}\underset{\sim}{n}})^{-1} \tag{B-9}$$

where

$$R_{\delta\underset{\sim}{k}\delta\underset{\sim}{k}} = E\left\{\delta\underset{\sim}{k}\delta\underset{\sim}{k}\right\} \tag{B-10}$$

and

*Throughout this discussion we assume that the expectation values of $\delta\underset{\sim}{k}$ and $\underset{\sim}{n}$ are zero. This condition is appropriate to our calculation since we have no a priori expectation for the values of $\delta\underset{\sim}{k}$ and $\underset{\sim}{n}$.

$$R_{\underset{\sim}{nn}} = E\left\{\underset{\sim}{nn}\right\} \tag{B-11}$$

Note that $R_{\underset{\sim}{nn}}$ and $R_{\underset{\sim}{\delta k}\underset{\sim}{\delta k}}$ are correlation matrices. In deriving Eq. B-9 we have assumed that $\underset{\sim}{\delta k}$ is completely uncorrelated with the $\underset{\sim}{n}$. Both $R_{\underset{\sim}{\delta k}\underset{\sim}{\delta k}}$ and $R_{\underset{\sim}{nn}}$ must be formed from our knowledge of what is acceptable in in $\underset{\sim}{\delta k}$ and $\underset{\sim}{n}$. Since the degree of correlation of two values of $\underset{\sim}{\delta k}$ is expected to decrease with increasing difference between the ξ_i's associated with the points, we take

$$(R_{\underset{\sim}{\delta k}\underset{\sim}{\delta k}})_{ij} = Ae^{-\left|i-j\right|/M} \tag{B-12}$$

where A is a constant (which will later drop out of the calculation); and M is a measure of how far the correlation between points extends.

Following Franklin[29] we consider $\underset{\sim}{n}$ to be due to round off error due to the finite arithmetic used in the machine calculation. We assume that the size of this error is approximately $10^{-d}\underset{\sim}{G\delta k}$ where d is the number of places of significance expected in the calculations and that the error is totally uncorrelated from point to point. Thus, we take

$$(R_{\underset{\sim}{nn}})_{ij} = 10^{-2d}\delta_{ij}(\underset{\sim}{G}R_{\underset{\sim}{\delta k}\underset{\sim}{\delta k}}\underset{\sim}{G}^T)_{ii} \tag{B-13}$$

With this choice of $R_{\underset{\sim}{nn}}$ the A of Eq. B-12 drops out completely. The final solution is unaffected by a range of choices of d(=1,2) and M(=3-6). The use of Eqs. B-9 and B-7 instead of solving Eq. B-4 directly

stabilizes the solution and allows it to reach the region of convergence without pushing the function into some unacceptable shape.

On the following pages, we have a listing of the Fortran source deck for this program:

```
C     MAIN PROGRAM FOR EVALUATION OF E-K FROM I-V DATA
C     PROGRAM MODIFIED TO SEARCH FOR BEST VALUE OF MS
C     MODIFIED TO COMPUTE STATISTICAL CORRELATIONS
C     OD=18-CHARACTER SAMPLE IDENTIFICATION
C     M=NO. OF DATA PTS.. AII,AIA=MIN.,MAX. LOG(I),VI,VA=MIN MAX V FOR
C     I-V PLOTTING
C     JO=EDIT CONTROL JO=1 EDIT     N2=ARRAY OF LOCATIONS OF EDITS
C     AI=CURRENT ARRAY,V=VOLTAGE ARRAY
C     N=ORDER OF INTERPOLATION,N+NOP= NO. OF PTS. USED IN INTERPOLATING
C     INPT=NO. OF PTS. USED THROUGHOUT THE CALCULATION
C     INPTI=NUMBER OF PTS BETWEEN V(1)AND VCO:INPTI=   <1  OPTION PASSED
C     J1=OUTPUT CONTROL J1=1 E-K,SQRT(E)-K,J1=2 SQRT(E)-K,J1=3E-K
C     J2=OUTPUT CONTROL J2=1 OUTPUT EACH ITERATION J2=2 ONLY LAST
C     ITERATION
C     EI,EA=MIN.,MAX. ENERGY. SEI,SEA=MIN.,MAX. SQRT(E),AKI,AKA=MIN
C     MAX. K FOR PLOTTING
C     NIT=MAX. NO. OF ITERATIONS,FUDGE = FUDGE FACTOR,AREA= AREA*10E-11
C     *A**2  THICK= THICKNESSIN A, ERRORK= ALLOWED K ERROR
C     ERRORI=ALLOWED INVERSION ERROR
C     PHI=BARRIER1,PH2=BARRIER2,ZI=MIN.ENERGY FORK VARIATION
C     ZA=MAX. ENERGY FOR K VARIATION
C     J3=PROGRAM CONTROL J3=1 RESTART,J3=2 N,NOP... ,J3=3 NIT,...
C     J3=4 PHI,PH2,...
C     J4=1 ERROR DATA ON EACH ITERATION,J5=1 PUNCH E-K,
C     J6=1 LIST DISTRIBUTIONS
C     ALKI,ALKA=MIN., MAX. VALUE OF K ALLOWED;
C     NCF= NUMBER O POINTS CORRELATED , ND= NUMBER OF PLACES OF
C     PRECISION
C     MSI,MSA= MIN., MAX. VALUES OF THE EFFECTIVE MASS
C     NMS= NUMBER OF DIFFERENT VALUES TO BE TRIED;NMS<=1 MSI =MS
      IMPLICIT REAL*8(A-H,O-Z)
```

```
      COMMON /KERNC/G(50,50),F(50,50),IL3(50)
      DIMENSION       N2(100),AI(100),V(100),VC(50),AILC(50) ,AIL(100),
     1Z1(150),AJ(50),AJC(50),DAK(50),AK1(150),E(50)
      DIMENSION AKERN(50,25),DJ(50),ATKER(50,25),SE(150),AJP(50),
     1AJCP(50),DIS(50),BT(50),R11(50,25),T1(50,25),T2(50,25)
      REAL AII,AIA,VI,VA,EI,EA,SEI,SEA,AKI,AKA,DD(5)
      DOUBLE PRECISION MSI,MSA,MST,MS
C     READ DATA AND EDIT
10    READ(5,1000) (DD(L0),L0=1,5)
1000  FORMAT(5A4)
20     READ(5,1010) M,AII,AIA,VI,VA,JO
1010  FORMAT (I10,4E10.3,I10)
      IF (JO .NE. 1) GO TO 30
      K1=8
25    READ(5,1015)N2(K1-7),N2(K1-6),N2(K1-5),N2(K1-4),N2(K1-3),N2(K1-2),
     1N2(K1-1),N2(K1)
1015  FORMAT (8I10)
      IF(N2(K1) .EQ. 0) GO TO 30
      K1=K1+8
      GO TO 25
30    READ(5,1020)(AI(L1),L1=1,M)
      READ(5,1020) (V(L2),L2=1,M)
1020  FORMAT(8D10.3)
      IF (JO .EQ. 1) CALL EDITIV(AI,V,N2,K1,M)
C     COMPUTE EQUAL INCREMENT IN V
      DO 40 L3=1,M
40    AIL(L3)=DLOG10(AI(L3))
C     READ DATA ON INTERPOLATION AND TOTAL NO. OF PTS.
50    READ(5,1030) N,NOP,INPT,INPT1,VCO
1030  FORMAT (4I10,D10.3)
      IF (INPT1 .LE. 1) VCO=V(I)
```

```
      IF (INPT1 .LE. 1) INPT1=1
      IF (INPT1 .LE. 1) GO TO 54
      DO 53 L41=1,INPT1
53    VC(L41)=V(1)+(VCO-V(1))*FLOAT(L41-1)/FLOAT(INPT1-1)
54    DO 55 L42=INPT1,INPT
55    VC(L42)=VCO+(V(M)-VCO)*FLOAT(L42-INPT1)/FLOAT(INPT-INPT1)
      DO 60 L4=1,INPT
60    E(L4)=V(M)*FLOAT(L4-1)/FLOAT(INPT-1)
      CALL INTERS(V,AIL,VC,AILC,N,M,INPT,NOP)
C     OUTPUT OF BASIC INFORMATION
      WRITE(6,2000) (DD(L100),L100=1,5)
2000  FORMAT(1H1,10HSAMPLE NO.,5X,5A4)
      WRITE(6,2010) N,M,NOP, INPT
2010  FORMAT(1HO,16HORDER OF POLFIT=,I2,10X,17HNO. OF DATA PTS.=,I3,10X,
     121HINTERPOLATION WITH N+,I3,2X,6HPOINTS,5X ,18HTOTAL NO. OF PTS.=,
     1I3)
      WRITE (6,2020)
2020  FORMAT(///1HO,3HNO.,17X,7HCURRENT,13X,7HVOLTAGE)
      WRITE(6,2030) (L5,AI(L5),V(L5),L5=1,M)
2030  FORMAT (1HO,I3,17X,D11.4,9X,D11.4)
C     BEGIN E-K COMPUTATION
C     READ PLOTTING INFORMATION
70    READ(5,1040) J1,J2,EI,EA,SEI,SEA,AKI,AKA
1040  FORMAT(2I10,6E10.3)
C     READ DATA ON SAMPLE AND CONTROL
80    READ(5,1050) NIT,FUDGE,AREA,THICK,ERRORK,ERRORI
1050  FORMAT(I10,5D10.3)
90    READ(5,1060) PH1,PH2,ZI,ZA,J3,J4,J5,J6
1060  FORMAT(4D10.3,4I10)
      READ(5,1070) ALKI,ALKA,NCF,ND ,EG,MSI,MSA,NMS
1070  FORMAT(2D10.3,2I10,3D10.3,I10)
```

```
      WRITE(6,2050) (DD(L101),L101=1,5)
2050  FORMAT (1H1,10HSAMPLE NO.,5X,5A4)
      WRITE(6,2060) PH1,PH2,THICK,AREA,FUDGE
2060  FORMAT (1HO,9HBARRIER1=,D10.3,5X,9HBARRIER2=,D10.3,5X,10HTHICKNESS
     1=,D10.3,5X,5HAREA=,D10.3,5X,6HFUDGE=,D10.3)
      WRITE(6,2070) ERRORK,INPT,NIT,J1,J2,J3
2070  FORMAT (1HO,7HERRORK=,D10.3,5X,16HNO. OF PTS. INT=,I3,5X,
     126HNO. OF ITERATIONS ALLOWED=,I3,5X,3HJ1=,I2,5X,3HJ2=,I2,5X,3HJ3=,
     1I2)
      WRITE(6,2076) INPT1,VCO,J4,J5,J6
2076  FORMAT (1HO,6HINPT1=,I3,5X,4HVCO=,D10.3,5X,3HJ4=,I2,5X,3HJ5=,I2,5X
     1,3HJ6=,I2)
      WRITE(6,2077) ALKI,ALKA,NCF,ND,EG,MSI,MSA,NMS
2077  FORMAT (1HO,5HALKI=,D10.3,5X,5HALKA=,D10.3,5X,4HNCF=,I2,5X,3HND=,
     1I2,//1X,11HENERGY GAP=,D10.3,5X,14HMS VARIED FROM,D10.3,2X,
     12HTO,D10.3,5X,4HWITH,I3,2X,6HVALUES)
      WRITE (6,2075) ZI,ZA
2075  FORMAT (1HO,13HK VARIED FORM ,3X,D10.3,3X,2HTO,3X,D10.3)
C     RENORMALIZATION OF CURRENT
      CI=6.1855D-5*FUDGE*AREA
      DO 100 L6=1,INPT
100   AJ(L6)=(10.0**AILC(L6))/(6.1855D5*FUDGE*AREA)*1.0D10
      DZ=(ZA-ZI)/FLOAT(INPT-1)
C     COMPUTATION OF Z1 ARRAY
C     LIMITS ON Z1 ARRAY
      IF((PH2 .GT. PH1) .AND. (VC(INPT) .LE.(PH2-PH1))) GO TO 120
      Z1I=PH2-VC(INPT)
      Z1A=PH1+VC(INPT)
      GO TO 130
120   Z1I=PH1
      Z1A=PH2
```

```
130   IF((Z1I.LE. ZI) .AND. (Z1A .GE. ZA)) GO TO 140
      WRITE(6,2040) Z1I,Z1A
2040  FORMAT (1HO,23HERROR IN LIMITS ON ZETA,5X,4HZII=,D10.3,5X,4HZ1A=,
     1D10.3)
      STOP
140   KB=1
150   IF (Z1I .GE. (ZI-FLOAT(KB)*DZ)) GO TO 160
      KB=KB+1
      GO TO 150
160   Z1(1)=ZI-FLOAT(KB-1)*DZ
      NZ1=1
170   IF ((Z1(NZ1)+DZ) .GE. Z1A) GO TO 180
      NZ1=NZ1+1
      Z1(NZ1)=Z1(1)+DZ*FLOAT(NZ1-1)
      GO TO 170
180   DO 182 L300=1,NZ1
182   SE(L300)=DSQRT(Z1(L300))
C     COMPUTATION OF R11
      CALL CORRLF(R11,INPT,NCF)
C     COMPUTATION OF EFFECTIVE MASS
      IF (NMS.LE. 1) GO TO 185
      ERRMF=1.0D+65
      DO 184 LM1=1,NMS
      MST=MSI+(MSA-MSI)*FLOAT(LM1-1)/FLOAT(NMS-1)
      CALL IMGUES(NZ1,Z1,AK1,MST,EG)
      CALL CURR(PH1,PH2,THICK,NZ1,INPT,AK1,Z1,VC,E,AJC)
      ERRM=0.0
      DO 183 LM2=1,INPT
183   ERRM=ERRM+DABS((AJC(LM2)-AJ(LM2))/AJ(LM2))
      IF (ERRM .GE. ERRMF) GO TO 184
      ERRMF=ERRM
```

```
      NMSL=LM1
184   CONTINUE
      MS=MSI+(MSA-MSI)*FLOAT(NMSL-1)/FLOAT(NMS-1)
      GO TO  186
185   MS=MSI
186    WRITE(6,8000) MS
8000  FORMAT(1HO,8HBEST MS=,D10.3)
      CALL IMGUES(NZ1,Z1,AK1,MS,EG)
      IF(J2 .NE. 1) GO TO 187
      CALL EKPRIN(NZ1,AK1,Z1,SE,DD,5,0,DAK,-1,0)
187   NIT1=0
190   CALL CURR(PH1,PH2,THICK,NZ1,INPT,AK1,Z1,VC,E,AJC)
      CALL KERN(PH1,PH2,THICK,AK1,Z1,NZ1,K8,E,VC,INPT,AKERN)
      DO 195 L60=1,INPT
      DO 195 L61=1,INPT
195   ATKER(L60,L61)=AKERN(L61,L60)
C     COMPUTE DJ
      DO 200 L8=1,INPT
200   DJ(L8)=AJ(L8)-AJC(L8)
C     COMPUTATION OF CORRECTION MATRIX
      CALL DMTY(R11,ATKER,INPT,T1)
      CALL DMTY(AKERN,T1,INPT,T2)
      DO 500 I50=1,INPT
500   T2(I50,I50)=(1.0+10.0**(-2*ND))*T2(I50,I50)
      CALL BNDINV(T2,INPT,DETERM,ERRORI,ITEST)
      NIT1=NIT1+1
      IF (ITEST .EQ. 0) GO TO 202
      WRITE (6,2080) ITEST,NIT1
2080  FORMAT (1H1,25HERROR IN INVERSION ITEST=,I3,5X,14HITERATION NO.=,
     1I3)
      CALL DEFAUL(INPT,AJC,ATKER,T2    ,DAK,ERRORC,0,C1,VC)
```

```
      STOP
202   CALL DMTY(T1,T2,INPT,AKERN)
      DO 203 L50=1,INPT
      DAK(L50)=0.0
      DO 203 L51=1,INPT
203   DAK(L50)=DAK(L50)+AKERN(L50,L51)*DJ(L51)
C     CHANGE IN VALUE OF K AND COMPUTATION OF ERROR
      ERRORC=0.0
      DO 204 L70=1,INPT
      IF (DABS(DAK(L70)) .GT. ERRORC) ERRORC=DABS(DAK(L70))
204   CONTINUE
      DO 210 L9=1,INPT
      LT=L9-1+K8
      IF ((AK1(LT)+DAK(L9)) .GT. ALKA) GO TO 206
      IF ((AK1(LT)+DAK(L9)) .LT. ALKI) GO TO 207
      AK1(LT)=AK1(LT)+DAK(L9)
      GO TO 210
206   AK1(LT)=ALKA
      GO TO 210
207   AK1(LT)=ALKI
210   CONTINUE
      IF ((ERRORC .LE. ERRORK) .OR. (NIT1 .GE. NIT)) GO TO 220
218   WRITE(6,2090) NIT1
2090  FORMAT (1H1,14HITERATION NO.=,I3)
      IF(J2 .EQ. 1) CALL EKPRIN(NZ1,AK1,Z1,SE,DD,5,0,DAK,INPT,K8)
      IF (J4 .EQ. 1) CALL DEFAUL(INPT,AJC,ATKER,AKERN,DAK,ERRORC,1,C1,VC
     1)
      GO TO 190
C     FINAL OUTPUT
220   IF  (ERRORC .GT. ERRORK) WRITE(6,2100) NIT1,ERRORC
2100  FORMAT (1H1,16HFINAL ITERATION=,I3,10X,16HDID NOT CONVERGE,5X
```

```
     17HERRORC=,D10.3)
      IF(ERRORC .LE. ERRORK) WRITE(6,2110) NIT1,ERRORC
2110  FORMAT (1H1,16HFINAL ITERATION=,I3,5X,7HERRORC=,D11.4)
224   CALL CURR(PH1,PH2,THICK,NZ1,INPT,AK1,Z1,VC,E,AJC)
C     OUTPUT I-V DATA
      DO 225 L60=1,INPT
      AJCP(L60)=6.1855D-5*FUDGE*AREA*AJC(L60)
225   AJP(L60)=6.1855D-5*FUDGE*AREA*AJ(L60)
      WRITE(6,2120)
2120  FORMAT (1HO/1HO,9HFINAL I-V)
      WRITE(6,2130)
2130  FORMAT (1HO/1HO,3HNO.,17X,7HVOLTAGE,13X,13HINPUT CURRENT,7X,14HOUT
     1PUT CURRENT)
      WRITE(6,2140) (L61,VC(L61),AJP(L61),AJCP(L61),L61=1,INPT)
2140  FORMAT (1HO,I3,17X,D11.4,9X,D11.4,9X,D11.4)
      IF ((J1 .GT. 3) .OR. (J1 .LT. 1)) GO TO 226
      CALL PLTIVL(M,V,AI,VI,VA,AII,AIA,0,0,11,1,DD,20,13H=INITIAL DATA,
     113,9.0,0)
      CALL PLTIVL(INPT,VC,AJP,VI,VA,AII,AIA,0,0,12,1,DD,0,12H=INTER. DAT
     1A,12,8.5,1)
      CALL PLTIVL(INPT,VC,AJCP,VI,VA,AII,AIA,1,0,5,1,DD,0,
     120H=FINAL CALC. CURRENT,20,8.0,1)
226   IF (J6 .NE. 1) GO TO 229
C     OUTPUT DISTRIBUTIONS
      WRITE(6,2150)
2150  FORMAT (1H1,35HCURRENT VERSUS ENERGY DISTRIBUTIONS)
      WRITE (6,2160)
2160  FORMAT(1HO/1HO,7HVOLTAGE,13X,6HENERGY,14X,12HDISTRIBUTION)
      DO 228 L62=1,INPT
      L64=IL3(L62)
      DO  227 L63=1,L64
```

```
227   DIS(L63)=6.1855D-5*FUDGE*AREA*G(L62,L63)/F(L62,L63)
      WRITE(6,2170) VC(L62),E(1),DIS(1)
2170  FORMAT (1HO/1HO,D11.4,9X,D11.4,9X,D11.4)
      IF (IL3(L62) .LE. 1) GO TO  228
      WRITE (6,2180) (E(L65),DIS(L65),L65=2,L64)
2180  FORMAT (1HO,20X,D11.4,9X,D11.4)
228   CONTINUE
229   WRITE (6,2190)
2190  FORMAT (1H1,9HFINAL E-K)
      CALL EKPRIN(NZ1,AK1,Z1,SE,DD,5,J5,DAK,INPT,KB)
      IF ((J1 .EQ.1) .OR. (J1 .EQ.3))
     1CALL EKPLOT(NZ1,AK1,Z1,AKI,AKA,EI,EA,1,0,2,1,DD,20,0)
      IF ((J1 .EQ. 1) .OR. (J1 .EQ. 2))
     1CALL EKPLOT(NZ1,AK1,SE,AKI,AKA,SEI,SEA,1,0,0,1,DD,20,1)
230   IF ((J3.GT. 3) .OR. (J3 .LE. 0)) STOP
      GO TO (10,50,80,90),J3
      END
```

```
      SUBROUTINE KERN(PH1,PH2,THICK,AK1,Z1,NZ1,KB,E,VC,INPT,AKERN)
C     SUBROUTINE TO EVALUATE AKERN MATRIX
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON /KERNC/G(50,50),F(50,50),IL3(50)
      DIMENSION AK1(NZ1),Z1(NZ1),E(INPT),VC(INPT),GA(60)
      DIMENSION AKERN(50,INPT)
C     CASE DETERMINATION
      DZ=Z1(2)-Z1(1)
      IF (PH1 .GE. PH2) GO TO 170
C     INITIATE LOOP V
      DO 160 L1=1,INPT
      NUM=IL3(L1)
      EV=(PH2-PH1-VC(L1))/THICK
      IF (VC(L1) .GT. ((PH2-PH1)/2.0)) GO TO 60
C     IN CASE 1
      DO 50 L2=1,INPT
      L3=KB+L2-1
      IF ((Z1(L3) .GE. PH1)  .AND. (Z1(L3) .LE. PH2)) GO TO 10
      AKERN(L1,L2) =0.0
      GO TO 50
10    DO 20 L4=1,NUM
*20   GA(L4)=(G(L1,L4)/(F(L1,L4)*EV))*(1.0/(AK1(L3)*AK1(L3)*F(L1,L4))-2.
     10)*DZ
      IF((Z1(L3) .GE. PH1) . AND.( Z1(L3) .LE. (PH1+VC(L1)))) GO TO 40
      IF((Z1(L3) .GE. (PH1+VC(L1))) .AND. (Z1(L3) .LE. (PH2-VC(L1))))
     1GO TO 30
      A1=Z1(L3)-PH2+VC(L1)
      A2=VC(L1)
      AKERN(L1,L2)=RINT(GA,E,A1,A2,NUM,3,0)
      GO TO 50
30    A1=0.0
```

```
      A2=VC(L1)
      AKERN(L1,L2)=RINT(GA,E,A1,A2,NUM,3,0)
      GO TO 50
40    A1=0.0
      A2=Z1(L3)-PH1
      AKERN(L1,L2)=RINT(GA,E,A1,A2,NUM,3,0)
50    CONTINUE
      GO TO 160
60    IF (VC(L1) .GT. (PH2-PH1)) GO TO 115
C     CASE 2
      DO 110 L2=1,INPT
      L3=KB+L2-1
      IF ((Z1(L3) .GE. PH1) .AND. (Z1(L3) .LE. PH2)) GO TO 70
      AKERN(L1,L2)=0.0
      GO TO 110
70    DO 80 L4=1,NUM
80    GA(L4)=(G(L1,L4)/(F(L1,L4)*EV))*(1.0/(AK1(L3)*AK1(L3)*F(L1,L4))
     1-2.0)*DZ
      IF ((Z1(L3) .GE. PH1) . AND. (Z1(L3) .LE. (PH2-VC(L1)))) GO TO 100
      IF ((Z1(L3) .GE. (PH2-VC(L1))) .AND. (Z1(L3) .LE. (PH1+VC(L1))))
     1GO TO 90
      A1=Z1(L3)-PH2+VC(L1)
      A2=VC(L1)
      AKERN(L1,L2)=RINT(GA,E,A1,A2,NUM,3,0)
      GO TO 110
90    A1=Z1(L3)-PH2+VC(L1)
      A2=Z1(L3)-PH1
      AKERN(L1,L2)=RINT(GA,E,A1,A2,NUM,3,0)
      GO TO 110
100   A1=0.0
      A2=Z1(L3)-PH1
```

```
      AKERN(L1,L2)=RINT(GA,E,A1,A2,NUM,3,0)
110   CONTINUE
      GO TO 160
C     CASE 3
115   DO 150 L2=1,INPT
      L3=KB+L2-1
      IF ((Z1(L3) .GE. (PH2-VC(L1))) .AND. (Z1(L3) .LE. (PH1+VC(L1))))
     1GO TO 120
      AKERN(L1,L2) =0.0
      GO TO 150
120   DO 125 L4=1,NUM
125   GA(L4)=(G(L1,L4)/(F(L1,L4)+EV))*(1.0/(AK1(L3)*AK1(L3)*F(L1,L4))
     1-2.0)*DZ
      IF ((Z1(L3) .GE. (PH2-VC(L1))) .AND. (Z1(L3) .LE. PH1)) GO TO 140
      IF ((Z1(L3) .GE. PH1) .AND. (Z1(L3) .LE. PH2)) GO TO 130
      A1=Z1(L3)-PH1
      A2=VC(L1)
      AKERN(L1,L2)=-RINT(GA,E,A1,A2,NUM,3,0)
      GO TO 150
130   A1=Z1(L3)-PH1
      A2=Z1(L3)-PH2+VC(L1)
      AKERN(L1,L2)=-RINT(GA,E,A1,A2,NUM,3,0)
      GO TO 150
140   A1=0.0
      A2=Z1(L3)-PH2+VC(L1)
      AKERN(L1,L2)=-RINT(GA,E,A1,A2,NUM,3,0)
150   CONTINUE
160   CONTINUE
      GO TO 220
C     CASE 4
170   DO 210 L1=1,INPT
```

```
      NUM=IL3(L1)
      EV=(PH2-PH1-VC(L1))/THICK
      DO 210 L2=1,INPT
      L3=KB+L2-1
      IF (Z1(L3) .GE. (PH2-VC(L1)) .AND. (Z1(L3).LE. (PH1+VC(L1))))
     1GO TO 180
      AKERN(L1,L2)=0.0
      GO TO 210
180   DO 175 L4=1,NUM
175   GA(L4)=(G(L1,L4)/(F(L1,L4)*EV))*(1.0/(AK1(L3)*AK1(L3)*F(L1,L4))
     1-2.0)*DZ
      IF((Z1(L3) .GE. (PH2-VC(L1))).AND. (Z1(L3) .LE. PH2)) GO TO 200
      IF ((Z1(L3) .GE. PH2) .AND. (Z1(L3) .LE. PH1)) GO TO 190
      A1=Z1(L3)-PH1
      A2=VC(L1)
      AKERN(L1,L2)=-RINT(GA,E,A1,A2,NUM,3,0)
      GO TO 210
190   A1=0.0
      A2=VC(L1)
      AKERN(L1,L2)=-RINT(GA,E,A1,A2,NUM,3,0)
      GO TO 210
200   A1=0.0
      A2=Z1(L3)-PH2+VC(L1)
      AKERN(L1,L2)=-RINT(GA,E,A1,A2,NUM,3,0)
210   CONTINUE
C     NOW TO MAKE SIMPSON RULE CORRECTION
220   IF (2*(INPT/2) .EQ. INPT) GO TO 250
C     ODD CASE
      DO 240 L4=1,INPT
      AKERN(L4,1)=AKERN(L4,1)/3.0
      LC=INPT-1
```

```
      DO 230 L5=2,LC,2
      AKERN(L4,L5)=4.0*AKERN(L4,L5)/3.0
230   AKERN(L4,L5+1)=2.0*AKERN(L4,L5+1)/3.0
240   AKERN(L4,INPT)=AKERN(L4,INPT)/2.0
      RETURN
C     EVEN CASE
250   DO 270 L6=1,INPT
      AKERN(L6,1)=AKERN(L6,1)/2.0
      AKERN(L6,2)=5.0*AKERN(L6,2)/6.0
      LC=INPT-1
      DO 260 L7=3,LC,2
      AKERN(L6,L7)=4.0*AKERN(L6,L7)/3.0
260   AKERN(L6,L7+1)=2.0*AKERN(L6,L7+1)/3.0
270   AKERN(L6,INPT)=AKERN(L6,INPT)/2.0
      RETURN
      END
```

```
      SUBROUTINE CURR(PH1,PH2,THICK,NZI,INPT,AK1,Z1,VC,E,AJC)
C     SUBROUTINE TO CALCULATE THE CURRENT AJC
C     NZI=DIMENSION OF AK1,Z1.INPT=DIMENSION OF VC,E,AJC
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION AK1(NZI),Z1(NZI),VC(INPT),E(INPT),AJC(INPT),AK1I(150)
     1,C(60)
      COMMON /KERNC/G(50,50),F(50,50),IL3(50)
C     COMPUTE G,FAND AJC
      DO 10 L1=1,NZI
10    AK1I(L1)=1.0/AK1(L1)
      DO 50 L2=1,INPT
      EV=(PH2-PH1-VC(L2))/THICK
      L3=0
20    L3=L3+1
      A1=PH1+E(L3)
      A2=PH2+E(L3)-VC(L2)
      T=-2.0*RINT(AK1,Z1,A1,A2,NZI,3,0)/EV+23.02585
      IF (DABS(T) .LT. 149.5) GO TO 22
      IF (T .GT. 0.0) G(L2,L3)=1.0D65
      IF ( T .LT. 0.0) G(L2,L3)=1.0D-65
      GO TO 25
22    G(L2,L3)=DEXP(T)
25    F(L2,L3)=RINT(AK1I,Z1,A1,A2,NZI,3,0)/EV
      IF((E(L3) .GT. VC(L2)) .OR. (L3 .GE. INPT)) GO TO 30
      GO TO 20
30    IL3(L2)=L3
      DO 40 L4=1,L3
40    C(L4)=G(L2,L4)/F(L2,L4)
      A2=VC(L2)
50    AJC(L2)=RINT(C,E,0.0,A2,L3,3,0)
      RETURN
      END
```

```
      SUBROUTINE INTERS(X,Y,XC,YC,NF,M1,M2,J1)
C     SUBROUTINE TO USE NF ORDER  INTERPOLATION TO COMPUTE ARRAY
C     OF YC(X)              GIVEN ARRAY Y(X).  M1=SIZE OF X ARRAY
C     M2=SIZE OF XC ARRAY . J1+N POINTS ARE USED IN THE INTERPOLATION
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION        X(100),Y(100),XC(100),YC(100),TX(31),TY(31),A(30)
      LOGICAL L1
C     DETERMINE THE ORDER IF  IT EXCEEDS  NUMBER OF PTS.
      IF ((NF +J1) .LE. M1) GO TO 8
      K=M1
      IF (NF .GT. M1) GO TO  6
      N=NF
      GO TO 10
6     N=M1-J1
      GO TO 10
8     N=NF
C     SEARCH FOR FIRST POINT
10    I=1
20    J=1
      IF (XC(I).LT. X(1)) GO TO 70
30    IF ((XC(I) .GE. X(J)) .AND.  (XC(I) .LE. X(J+1))) GO TO 35
      IF ((J+1) .GE. M1) GO TO 90
      J=J+1
      GO TO 30
35    L1=.FALSE.
      IF ((NF+J1) .LE. M1) K=N+J1
      IF (((K/2)*2-K) .EQ. 0) L1=.TRUE.
      IF (L1 .AND. ((J-K/2) .LT. 0)) GO TO 70
      IF (L1 .AND. ((J+K/2) .GT. M1)) GO TO 90
      IF ((.NOT. L1) .AND. ((J+(K+1)/2) .GT. M1)) GO TO 90
      IF ((.NOT. L1) .AND. ((J-(K-1)/2) .LT. 0)) GO TO 70
```

```
      IF (L1) GO TO 50
      DO 40 N2=1,K
      N1=J-(K-1)/2+N2
      TX(N2)=X(N1)
40    TY(N2)=Y(N1)
      GO TO 110
50    DO 60 N2=1,K
      N1=J-K/2+N2
      TX(N2)=X(N1)
60    TY(N2)=Y(N1)
      GO TO 110
C     NEAR BOTTOM
70    DO 80 N3=1,K
      TX(N3)=X(N3)
80    TY(N3)=Y(N3)
      GO TO 110
C     NEAR TOP
90    DO 100 N4=1,K
      N5=M1-K+N4
      TX(N4)=X(N5)
100   TY(N4)=Y(N5)
110   CALL DPOLIT(TX,TY,K,N,A)
C     CALCULATION OF VALUES
      N6=N-1
120   YC(I)=A(1)+A(N)*(XC(I)**(N-1))
      IF (N .LE. 2) GO TO  140
      DO 130 N7=2,N6
130   YC(I)=YC(I)+A(N7)*(XC(I)**(N7-1))
140   I=I+1
      IF ( I .GT. M2) RETURN
      IF ((XC(I) .GT. X(J+1)) .OR. (XC(I).LT. X(J))) GO TO 20


      GO TO 120
      END
```

```
      DOUBLE PRECISION FUNCTION RINT(F,X,A1,A2,N,MF,J)
C     FUNCTION TO COMPUTE THE INTEGRAL OF F(X) FROM A1 TO A2
C     N=SIZE OF F AND X ARRAYS
C     MF=ORDER OF POLYNOMINAL USED IN FIT  MF+J= NO. OF PTS.
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION F(N),X(N),A(30),TF(40),TX(40)
      IF ((MF+J).LE. N) GO TO 8
      K=N
      IF(MF .GT. N) GO TO 6
      M=MF
      GO TO 9
6     M=N-J
      GO TO 9
8     M=MF
9     IF (A1 .NE. A2) GO TO 10
      RINT=0.0
      RETURN
10    IF(A1 .GT. A2) GO TO 20
      X1=A1
      X2=A2
      GO TO 30
20    X1=A2
      X2=A1
30    IF((X1 .GT. (2.0*X(1)-X(2))).AND. (X2.LE. (2.0*X(N)-X(N-1))))
     1GO TO 40
      RINT=0.0
      WRITE(6,2000) X1,X2,X(1),X(N)
2000  FORMAT (1HO,23HERROR IN LIMITS IN RINT,5X,11HLIMITS FROM,D10.3,2X,
     12HTO,D10.3,5X,12HALLOWED FROM,D10.3,2X,2HTO,D10.3)
      RETURN
C     NOW TO COMPUTE THE INTERVAL
```

```
40    I1=1
45    IF ((X(I1).GE. X1) .OR. (I1 .GE. N)) GO TO 50
      I1=I1+1
      GO TO 45
50    I2=1
60    IF (((X(I2) .LE. X2) .AND. (X(I2+1) .GT. X2)) .OR.  ((I2+1) .GE. N
     1 )) GO TO 70
      I2=I2+1
      GO TO 60
70    IF (((I2+1) .GE. N) .AND. (X(I2+1) .LE. X2)) I2=I2+1
C     NOW TO COMPUTE ARRAYS AND INTEGRATE
      IF ((MF+J).LE. N)  K=M+J
      RINT=0.0
      IF (I2 .EQ. I1) GO TO 165
       IF (I2 .LT. I1) GO TO 172
      L2=I2-1
      DO 160 L1=I1,L2
      IF (L1 .LT. (K/2)) GO TO 110
      IF (2*(K/2) .EQ. K) GO TO 80
      IF ((N-L1) .LT. ((K+1)/2)) GO TO 130
      GO TO 90
C     EVEN
80    IF((N-L1) .LT. (K/2)) GO TO 130
C     IN MIDDLE
90    DO 100 L3=1,K
      LC=L1-(K/2)+L3
      TF(L3)=F(LC)
100   TX(L3)=X(LC)
      GO TO 145
C     NEAR BEGINNING
110   DO 120 L4=1,K
```

```
      TF(L4)=F(L4)
120   TX(L4)=X(L4)
      GO TO 145
C     NEAR END
130   DO 140 L5=1,K
      LCC=L5+N-K
      TF(L5)=F(LCC)
140   TX(L5)=X(LCC)
145   CALL DPOLIT(TX,TF,K,M,A)
      DO 150 L6=1,M
150   RINT=RINT+A(L6)*(X(L1+1)**L6-X(L1)**L6)/FLOAT(L6)
160   CONTINUE
C     CORRECTION FOR END PTS.
165   IF (X1 .EQ. X(I1)) GO TO 170
      IA=I1
      IF (I1 .GT. 1) IT=I1-1
      IF( I1 .EQ. 1) IT=I1
      JC=1
      GO TO 180
170   IF (X2 .EQ. X(I2)) GO TO 300
      IT=I2
      JC=2
      GO TO 180
172   IT=I2
      JC=3
180   IF (IT .LT. (K/2)) GO TO 220
      IF (2*(K/2) .EQ. K) GO TO 190
      IF ((N-IT) .LT. ((K+1)/2)) GO TO  240
      GO TO 200
190   IF ((N-IT) .LT. (K/2)) GO TO 240
200   DO 210 L7=1,K
```

```
      LC=IT-(K/2)+L7
      TF(L7)=F(LC)
210   TX(L7)=X(LC)
      GO TO 260
220   DO 230 L8=1,K
      TF(L8)=F(L8)
230   TX(L8)=X(L8)
      GO TO 260
240   DO 250 L9=1,K
      LCC=L9+N-K
      TF(L9)=F(LCC)
250   TX(L9)=X(LCC)
260   CALL DPOLIT(TX,TF,K,M,A)
      IF (JC.EQ. 3) GO TO 292
      IF (JC .EQ. 2) GO TO 280
      DO 270 L10=1,M
270   RINT=RINT+A(L10)*(X(IA)**L10-X1**L10)/FLOAT(L10)
      GO TO 170
280   DO 290 L11=1,M
290   RINT=RINT+A(L11)*(X2**L11-X(IT)**L11)/FLOAT(L11)
      GO TO 300
292   DO 295 L12=1,M
295   RINT=RINT+A(L12)*(X2**L12-X1**L12)/FLOAT(L12)
300   IF (A1 .GT. A2) RINT=-RINT
      RETURN
      END
```

```
      SUBROUTINE DMTY(A,B,N,C)
C     MATRIX MULTIPLIER C=AB
C     N=SIZE OF MATRIX
      DOUBLE PRECISION A(50,N),B(50,N),C(50,N)
      DO 10 L1=1,N
      DO 10 L2=1,N
      C(L1,L2)=0.0
      DO 10 L3=1,N
10    C(L1,L2)=C(L1,L2)+A(L1,L3)*B(L3,L2)
      RETURN
      END
```

```
      SUBROUTINE CORRLF(R,N,NCF)
      DOUBLE PRECISION R(50,N)
      DO 10 L1=1,N
      DO 10 L2=1,N
10    R(L1,L2)=EXP(-ABS(FLOAT(L1-L2))/FLOAT(NCF))
      RETURN
      END
```

```
      SUBROUTINE IMGUES(NZ1,Z1,AK1,MS,EG)
C     SUBROUTINE TO COMPUTE ARRAY AK1=SQRT(Z1*(EG-Z1))/(H8*SQRT(EG/(2*M*
C     ))
C     MS=M*
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION Z1(NZ1),AK1(NZ1)
      DOUBLE PRECISION MS
      DO 10 L1=1,NZ1
      IF((Z1(L1) .LE. 0.0) .OR. (Z1(L1) .GE. EG)) GO TO 5
      AK1(L1)=0.5125*DSQRT(MS)*DSQRT(Z1(L1)*(EG-Z1(L1))/EG)
      GO TO 10
5     AK1(L1)=-0.5125*DSQRT(MS)*DSQRT(DABS(Z1(L1)*(EG-Z1(L1))/EG))
10    CONTINUE
      RETURN
      END
```

```
      SUBROUTINE DPOLIT(X,Y,M,N,A)
C     SUBROUTINE TO MAKE POLY FIT TO FUNCTION DEFINED BY Y(X),
C     M= NO. OF DATA PTS., N= ORDER OF POLY.
      DOUBLE PRECISION X(150),Y(150),A(30),B(30,30),C(150),C1(150),
     1C2(150),C3(150),C4(150),C5(30),T1,D,BE,GA,AL
C     COMPUTE THE POLY UP TO DEGREE N
      IF (N .GT. M) GO TO 080
      DO 010 L1=1,M
010   C(L1)=1.0
      B(1,1)=1.0/SQRT(FLOAT(M))
      IF (N .LE. 1) GO TO 045
      T1=DSQRT(D(X,X,M)-((D(C,X,M))**2)/FLOAT(M))
      B(2,2)=1.0/T1
      B(2,1)=-D(X,C,M)/(FLOAT(M)*T1)
      IF (N .LE. 2) GO TO 045
C     COMPUTE OTHER POLY. N.GT. 2
      DO 040 L2=3,N
      DO 035 L3=1,M
      C1(L3)=B(L2-1,1)
      C2(L3)=0.0
      C3(L3)=B(L2-2,1)
      L100=L2-1
      DO 020 L4=2,L100
020   C1(L3)=C1(L3)+B(L2-1,L4)*(X(L3)**(L4-1))
      C2(L3)=X(L3)*C1(L3)
      L101=L2-2
      IF (L101 .LT. 2 ) GO TO 035
      DO 030 L5=2,L101
030   C3(L3)=C3(L3)+B(L2-2,L5)*(X(L3)**(L5-1))
035   CONTINUE
C     NOW ALL INFORMATION NECESSARY FOR GENERATING FUNCTIONS ARE
```

```
C     AVAILABLE
      BE=-D(C1,C2,M)
      GA=-D(C2,C3,M)
      AL=1.0/DSQRT(D(C2,C2,M)-BE*BE-GA*GA)
      B(L2,1)=AL*(BE*B(L2-1,1)+GA*B(L2-2,1))
      B(L2,L2-1)=AL*(B(L2-1,L2-2)+BE*B(L2 -1,L2-1))
      B(L2,L2)=AL*B(L2-1,L2-1)
      IF (L101 .LT. 2) GO TO 40
      DO 038 L6=2,L101
038   B(L2,L6)=AL*(B(L2-1,L6-1)+BE*B(L2-1,L6)+GA*B(L2-2,L6))
040   CONTINUE
C     FITTING OF FUNCTION TO POLY.
045   DO 060 L7=1,N
      DO 051 L8=1,M
      C4(L8)=B(L7,1)
      IF (L7 .EQ. 1) GO TO 051
      DO 050 L9=2,L7
050   C4(L8)=C4(L8)+B(L7,L9)*(X(L8)**(L9-1))
051   CONTINUE
060   C5(L7)=D(Y,C4,M)
      DO 070 L10=1,N
      A(L10)=0.0
      DO 070 L11=L10,N
070   A(L10)=A(L10)+B(L11,L10)*C5(L11)
      RETURN
080   WRITE (6,1000)
1000  FORMAT (1H0,25HN .GT. M FIT NOT EXECUTED)
      RETURN
      END
      DOUBLE PRECISION FUNCTION D(X,Y,M)
      DOUBLE PRECISION X(150),Y(150)


      D=0.0
      DO 010 L1=1,M
010   D=D+X(L1)*Y(L1)
      RETURN
      END
```

```
      SUBROUTINE EDITIV(AI,V,N,K,M)
C     SUBROUTINE TO EDIT IN PUT DATA OFF OF CARDS
C     AI=INPUT ARRAY OF CURRENTS,V=INPUT VOLTAGE ARRAY,N=INPUT NO. ARRAY
C     OF LOCATIONS OF DELETIONS,K=NO. OF ELEMENTS IN N,M= NO. OF
C     ORIGINAL DATA PTS.  MODIFIED BY PROGRAM
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION AI(100),V(100),N(100)
      IF (K .EQ. 0) RETURN
      DO 30 L1=1,K
      IF ((N(L1) .LE. 0) .OR. (N(L1) .GT. M)) GO TO  30
      L2=N(L1)
      M=M-1
      DO 10 L3=L2,M
      AI(L3)=AI(L3+1)
10    V(L3)=V(L3+1)
      L4=L1+1
      DO 20 L5=L4,K
20    N(L5)=N(L5)-1
30    CONTINUE
      RETURN
      END
```

```
      SUBROUTINE PLTIVL(N,V,AI,VI,VA,AIIL,AIAL,LAB,IP,ISYS,ISP,DD,M1,DC,
     1M2,YS,M3)
C     SUBROUTINE TO PLOT I-V CURVE ON LOG-LINEAR PAPER
C     N=NUMBER OF POINTS;V=VOLTAGE ARRAY,AI=CURRENT ARRAY
C     AIIL,AIAL=LIMITS ON LOG CURRENT: VI,VA=LIMITS ON VOLTAGE
C     DD=SAMPLE NAME ARRAY;M1=LENGTH OF DD;DC=CHARACTER IDENTIFICATION ;
C     M2=LENGTH OF DC
C     YS=Y LOCATION OF DC,M3=1 SKIP LABEL
      DOUBLE PRECISION V(N),AI(N)
      DIMENSION DD(5),DC(5),VP(100),AIP(100),DQ(3)
      COMMON /COMPXY/ITEST,XLNGTH,YLNGTH
      ITEST=1
      XLNGTH=14.0
      YLNGTH=10.0
      DQ(1)=0.0
      DQ(3)=1.0
      DO 10 L1=1,N
      VP(L1)=V(L1)
10    AIP(L1)=DLOG10(AI(L1))
      IF (M1.LE. 0) GO TO 20
      CALL SYSSYM(11.5,9.5,.25,DD,M1,0.0)
20    IF (M2 .LE. 0) GO TO 30
      CALL SYSSYM(11.5,YS,.25,ISYS,-1,0.0)
      CALL SYSSYM(11.75,YS,.25,DC,M2,0.0)
30    IF (M3 .EQ. 1) GO TO  40
      CALL LABEL (0.0,0.0,VI,VA,14.0,7,16HVOLTAGE IN VOLTS,16,0)
      CALL LABEL (0.0,0.0,AIIL,AIAL,10.0,5,11HLOG CURRENT,11,1)
40    CALL PLOTXY(N,VP,AIP,VI,VA,    AIIL,AIAL,LAB,IP,ISYS,ISP,DQ)
      RETURN
      END
```

```
      SUBROUTINE EXPRIN(N,AK,E,SE,DD,M1,M2,DAK,NA,KB)
C     SUBROUTINE TO OUTPUT E-K DATA
C     N=NUMBER OF PTS.;AK=K-ARRAY;E=ENERGY ARRAY;SE=SQRT(E) ARRAY
C     DD= SAMPLE IDENTIFICATION
C     M1=SIZE OF DD ARRAY;M2=1 PUNCH E-K DATA
C     DAK=VARIATION IN K ARRAY;NA= NUMBER OF POINTS;
C     KB=LOCATION OF FIRST POINT;NA<0 NO DAK'S
      DOUBLE PRECISION AK(N),E(N),SE(N),DAK(50),DAKO(100),AK2(100)
      DO 20 L1=1,N
      AK2(L1)=AK(L1)**2
      IF (NA .LE. 0) GO TO 10
      IF ((L1 .LT. KB) .OR. (L1 .GT. (KB+NA-1))) GO TO 10
      L2=L1+1-KB
      DAKO(L1)=DAK(L2)
      GO TO 20
10    DAKO(L1)=0.0
20    CONTINUE
      DIMENSION DD(M1)
      WRITE(6,2000)
2000  FORMAT (1H0/1H0,3HNO.,17X,6HENERGY,14X,7HSQRT(E),13X,1HK,19X,
     14HK**2,16X,3HDAK)
      WRITE (6,2010) (L1,E(L1),SE(L1),AK(L1),AK2(L1),DAKO(L1),L1=1,N)
2010  FORMAT (1H0,I3,17X,D11.4,9X,D11.4,9X,D11.4,9X,D11.4,9X,D11.4)
      IF (M2 .NE. 1) RETURN
      PUNCH 2020,(DD(L2),L2=1,M1)
2020  FORMAT (20A4)
      PUNCH 2030,N
2030  FORMAT (I10)
      PUNCH 2040,(E(L3),L3=1,N)
      PUNCH 2040,(AK(L4),L4=1,N)
2040  FORMAT (8D10.3)
      RETRUN
      END
```

```
      SUBROUTINE DEFAUL(INPT,AJC,AKERN,AKERNI,DAK,ERRORC,M,C1,VC)
C     SUBROUTINE TO GIVE ERROR OUTPUT
C     M=1 PRINT DAK,ERRORC
C     INPT=SIZE OF AJC,AKERN,AKERNI,G,F,DAK ARRAYS
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON/KERNC/G(50,50),F(50,50),IL3(50)
      DIMENSION AJC(INPT),AKERN(50,INPT),AKERNI(50,INPT),DAK(INPT)
      DIMENSION VC(INPT),AJO(50)
      DO 5 LO=1,INPT
5     AJO(LO)=C1*AJC(LO)
      WRITE(6,2000)
2000  FORMAT (1HO/1HO,16HERROR CHECK DATA)
      WRITE(6,2010)
2010  FORMAT(1HO,25HDISTRIBUTIONS AND CURRENT)
      DO 10 L1=1,INPT
      WRITE (6,2020) L1,L1
2020  FORMAT(1HO,2HL2,18X,2HG(,I2,4H,L2),12X,2HF(,I2,4H,L2))
      IK=IL3(L1)
      WRITE(6,2030) (L2,G(L1,L2),F(L1,L2),L2=1,IK)
2030  FORMAT (1H ,I3,17X,D11.4,9X,D11.4)
10    WRITE (6,2040) L1,AJO(L1),L1,VC(L1)
2040  FORMAT (1HO,4HAJC(,I2,2H)=,D11.4,5X,3HVC(,I2,2H)=,D11.4)
      WRITE (6,2050)
2050  FORMAT (1H1,25HMATRICES AKERN AND AKERNI)
      DO  20 L3=1,INPT
      WRITE (6,2060) L3
2060  FORMAT (1HO,3HROW,I3,5X,5HAKERN)
20    WRITE(6,2070) (AKERN(L3,L4),L4=1,INPT)
2070  FORMAT (1H ,10D13.3)
      DO 30 L5=1,INPT
      WRITE(6,2080) L5

2080  FORMAT (1HO,3HROW,I3,5X,6HAKERNI)
30    WRITE(6,2070) (AKERNI(L5,L6),L6=1,INPT)
      IF (M .NE. 1) RETURN
      WRITE(6,2090)
2090  FORMAT (1HO/1HO,3HNO.,5X,3HDAK)
      WRITE(6,2100) (L7,DAK(L7),L7=1,INPT)
2100  FORMAT (1H ,I3,5X,D11.4)
      WRITE(6,2110) ERRORC
2110  FORMAT (1HO/1HO,7HERRORC=,D11.4)
      RETURN
      END
```

```
      SUBROUTINE EKPLOT(N,AK,E,AKI,AKA,EI,EA,LAB,IP,ISYS,ISP,DD,M1,M2)
C     SUBROUTINE TO PLOT E-K OR SQRT(E)-K CURVES
C     N=NUMBER OF PTS.;AK=K-ARRAY;E=ENERGY OR SQRT(E) ARRAY
C     AKI,AKA=LIMITS OF K
C     EI,EA=LIMITS OF ENERGY,OR SQRT(E)
C     DD=SAMPLE NAME;M1=LENGTH OF DD
C     M2=1 SQRT(E) PLOT
      DOUBLE PRECISION AK(N),E(N)
      DIMENSION DD(5),AKP(100),EP(100),DQ(3)
      COMMON /COMPXY/ITEST,XLNGTH,YLNGTH
      ITEST=1
      XLNGTH=14.0
      YLNGTH=10.0
      DQ(1)=0.0
      DQ(3)=1.0
      DO 10 L1=1,N
      AKP(L1)=AK(L1)
10    EP(L1)=E(L1)
      CALL SYSSYM(11.5,9.5,.25,DD,M1,0.0)
      IF (M2 .EQ. 1) CALL LABEL (0.0,0.0,EI,EA,10.0,5,
     119HSQRT(E) IN SQRT(EV),19,1)
      IF (M2 .NE. 1) CALL LABEL(0.0,0.0,EI,EA,10.0,5,12HENERGY IN EV,12,
     11)
      CALL LABEL(0.0,0.0,AKI,AKA,14.0,7,8HK IN 1/A,8,0)
      CALL PLOTXY(N,AKP,EP,AKI,AKA,EI,EA,LAB,IP,ISYS,ISP,DQ)
      RETURN
      END
```

REFERENCES

1. M. McColl and C. A. Mead, Transactions of the Metallurgical Society of AIME 233, 502 (1964).

2. M McColl, "Electron Current Through Thin Mica Films" (unpublished Ph.D. dissertation, California Institute of Technology, (1964).

3. G. Lewicki and C. A. Mead, J. Phys. Chem. Solids 29, 1255 (1968).

4. G. Lewicki, "Electron Tunneling Through Thin Films of Aluminum Nitride" (unpublished Ph.D. dissertation, California Institute of Technology, 1966).

5. F. A. Padovani and R. Stratton, Solid-State Electron. 9, 695 (1966).

6. M. F. Millea, M. McColl, and C. A. Mead, Phys. Rev. 177, 1164 (1969).

7. G. H. Parker and C. A. Mead, Phys. Rev. Letters 21, 605 (1968).

8. G. H. Parker and C. A. Mead, Phys. Rev. (to be published).

9. E. O. Kane, J. Phys. Chem. Solids 12, 181 (1959).

10. V. Heine, Proc. Phys. Soc. (London) 81, 300 (1963).

11. R. O. Jones, Proc. Phys. Soc. (London) 89, 443 (1966).

12. E. I. Blount, Solid State Physics (Academic Press, New York, 1962), Vol. 13, Appendix C, p. 362.

13. N. H. Fletcher, Proc. Phys. Soc. (London) 91, 724 (1967).

14. N. H. Fletcher, Proc. Phys. Soc. (London) 92, 265 (1967).

15. P. Phariseau and J. M. Ziman, Phil. Mag. 8, 1487 (1963).

16. W. Harrison, Phys. Rev. 123, 85 (1961).

17. C. B. Duke, Tunneling Phenomena in Solids (Plenium Press, New York, 1969), Chap.4.

18. T. E. Feuchtwang, "The Generalized WKB Approximation for a Smooth Transition Between Two Different One-dimensional Periodic Potentials", Part I and II, (Submitted for publication to Phys. Rev.).

19. L. Esaki and P. J. Stiles, Phys. Rev. Letters 14, 902 (1965).

20. H. A. Antosiewicz and W. C. Rheinboldt, Survey of Numerical Analysis (McGraw-Hill Book Company, New York, 1962), Chap. 14, pp. 512-517.

21. K. K. Thornber, Thomas C. McGill and C. A. Mead, J. Appl. Phys. 38, 2384 (1967).

22. J. G. Simmons, Phys. Letters 16, 233 (1965).

23. C. A. Mead, E. H. Snow and B. E. Deal, Appl. Phys. Letters 9, 53 (1966).

24. C. B. Duke, Solid-State Physics (Academic Press, New York, to be published).

25. Richard Williams and Richard H. Bube, J. Appl. Phys. 31, 968 (1960).

26. R. M. Hill, Thin Solid Films 1, 39 (1967).

27. C. A. Mead, Phys. Rev. 128, 2088 (1962).

28. R. Stratton, G. Lewicki and C. A. Mead, J. Phys. Chem. Solids 27, 1599 (1966).

29. J. N. Franklin, "Well-Posed Stochastic Extensions of Ill-Posed Linear Problems", (to be published).