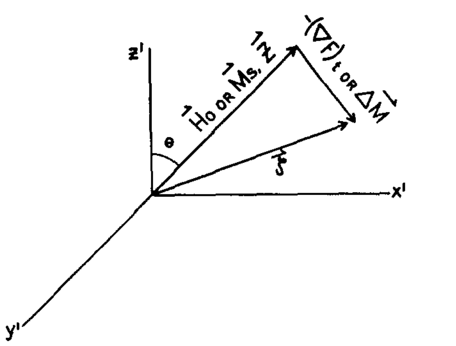

FIG. 1. Choice of axes; x', y', z' are cube edges.

are still a natural description of the medium along the 100 axis and the 111 axis, but not for the 110 axis or other angles.

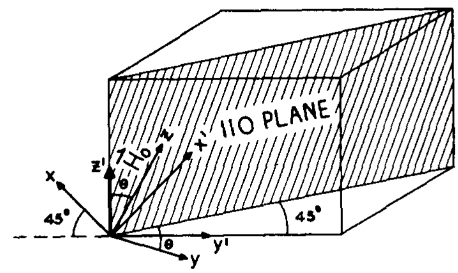

FIG. 2. 110 plane in cubic crystal. zy lies in 110 plane. H_0 lies along z. x', y', z' are cube edges

We note the Hermitian character of the tensor χ'. This is consistent with the time-reversal property of precession of the magnetization for a lossless situation.

We should like to express our thanks to R. C. LeCraw for bringing this problem to our attention.

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Exact Current-Voltage Relation for the Metal-Insulator-Metal Junction with a Simple Model for Trapping of Charge Carriers*

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The exact solution to the diffusion equation for one kind of charge carrier is obtained for the metal-insulator-metal junction where trapping of the charge carriers may occur in the body of the insulator. The effect of surface states is not considered. The electric potential distribution is given in closed form and the exact dc current-voltage relation is given in parametric form for any degree of trapping. A graph of the current-voltage relation is shown for the special case where the two boundary metals are the same.

A brief description of some experimental difficulties is given when test junctions were prepared entirely by the vacuum evaporation method.

INTRODUCTION

APPROXIMATE solutions to the diffusion equation have been published by Mott[1] for the case of the purely chemical barrier layer metal-semiconductor junction where the electric field in the barrier layer is essentially constant, and by Mott and Gurney[2] for the case of the metal-insulator contact where the change in field strength F in the insulator of thickness L is of the order F/L and where $F/L \ll eF^2/kT$. Shockley and Prim[3] obtain approximate solutions applied to the analogous physical situation of the p-intrinsic-p and n-intrinsic-n junctions for semiconductors showing the Child's law analog for semiconductors in the space charge limited region of the current-voltage characteristic. More recently, Skinner[4] discussed the properties of the metal-insulator contact and obtained an exact solution for the potential distribution within the insulator and a low current approximation of the current-voltage relation which predicts the possibility of a turn-over point (a negative resistance region) in the current-voltage relation.

This work extends the exact solution to include trapping of charge carriers. Also, the exact calculation of the entire range of the current-voltage relation is obtained with any degree of space charge effects. The solution obtained here applies also to the purely chemical barrier metal-semiconductor contact and the p-intrinsic-p or n-intrinsic-n junction. Torrey and Whitmer[5] had suggested the possibility of employing the metal-insulator-metal junction as an effective rectifier. Also Mott and Gurney suggested that space charge trapping may be an essential factor in the passage of charge carriers from a metal into an insulator. The further exploration of these two suggestions is contained in this work.

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MODEL OF THE JUNCTION

The model of the metal-insulator-metal contact is essentially that of the purely chemical barrier layer metal-semiconductor contact treated by Mott, or the n-intrinsic-n junction treated by Shockley and Prim. The barrier layer is an electrically neutral insulating crystal into which charge carriers of only one type (electrons in this treatment) are injected by thermionic emission from the metals at the boundaries. Electrons may enter and leave the insulator only at energies falling within the conduction band of the insulator. The concentration, n_c, of electrons in the conduction band adjacent to the metal is fixed at a value such that thermal equilibrium is maintained across the metal-insulator surface. The mean free path of the conduction band electrons is taken to be small compared to the thickness of the insulator. Conduction is by simple diffusion and drift alone rather than by tunneling or avalanches. Acceptor trap levels in the form of crystal defects may exist below and close to the conduction band and are assumed to be evenly distributed in space. The effect of surface state trapping is neglected and it is here that this model may be deficient. However, the effects of surface trapping can be distinguished experimentally from the effects of body trapping by measuring the resistivity of different thicknesses of the same insulator at constant applied electric field. The effect of the space charge is to resist the introduction of new charge carriers from the metal. If the space charge is trapped throughout the body of the material, then by reducing the thickness of the insulator one also reduces the number of traps and hence the space charge. This leads to an apparent reduction in the resistivity of the insulator. In contradistinction, the number of surface traps are not reduced by reducing the thickness of the insulator so an apparent increase in the resistivity would be noticed. Only if space charge effects of either kind are so small as to be of no consequence (or if by chance the effects should just balance) would the resistivity be unchanged. It is reasonable to assume that the rate of trapping R_t of conduction band electrons is proportional to the product of the conduction band electron concentration and the concentration of empty traps,

$$R_t = C_t n_c (d_t - n_t),$$

where d_t is the concentration of traps, n_t is the concentration of trapped electrons, and C_t is a constant. The rate of breaking free again, R_f, is proportional to the concentration of electrons in the trap levels

$$R_f = C_f n_t$$

where C_f is a constant. For equilibrium R_f is set equal to R_t to obtain

$$n_c = C_f n_t / C_t (d_t - n_t).$$

Assuming that $n_t \ll d_t$ (Boltzmann statistics apply to the carriers in the trap and conduction band levels), one has

$$n_c + n_t = p n_c,$$

where p, the "trapping factor," is equal to $(1+C_t d_t/C_f)$. Thus, the trapping model requires that a fixed fraction $1/p$ of the total charge carrier density at a given position in the insulator resides in the conduction band while the remainder resides in the traps.

POTENTIAL DISTRIBUTION AND CURRENT-VOLTAGE RELATION

Let the contact surfaces be plane with metal number zero in the region $x<0$, metal number one in the region $x>L$, and the insulator in the region $0\leq x\leq L$.

To determine the potential distribution within the barrier and the current-voltage relation one must obtain the simultaneous solution to the diffusion equation,

$$j = -De(dn_c/dx) - n_c eu(d\phi/dx),$$

the Poisson equation,

$$d^2\phi/dx^2 = -4\pi p n_c e/K,$$

and the continuity equation for the steady state,

$$dj/dx = 0,$$

where j is the electric current density, which clearly is not a function of x, D is the diffusion coefficient, e is the charge of the electron, u is the mobility, ϕ is the electric potential, and K is the dielectric constant.

At the boundaries one has $pn(0)=pn_0$ and $pn(L)=pn_1$. The quantities pn_0 and pn_1 are determined by the thermal equilibrium conditions at the boundaries and are taken to be independent of the current. In addition one has $\phi(L)-\phi(0)=\Delta\phi$ where $\Delta\phi$ is the contact potential plus the applied potential difference across the barrier.

Changing to the dimensionless variables,

$$q = x/L,$$
$$U = e\phi/kT,$$
$$Q = j2\pi L^3 ep/KDkT,$$

making use of the Einstein relation, $u/D=e/kT$, and eliminating n_c from the diffusion equation by use of the Poisson equation, one obtains

$$2Q = U''' + U''U', \qquad (1)$$

where the primes denote differentiation with respect to q. The boundary conditions are then expressed by

$$U_0'' = -4\pi pe^2 n_c(0)/kTK,$$
$$U_1'' = -4\pi pe^2 n_c(L)/kTK,$$

and

$$\Delta U = (e/kT)[\phi(L) - \phi(0)].$$

The consequences of the trapping model may be seen from the form of the dimensionless variables. Notice that p always occurs in conjunction with K as the ratio p/K. Hence, one may define an effective dielectric constant $K_{eff}=K/p$. Thus, the effect of trapping may be thought of mathematically as a change in the dielectric constant of the insulator. The properties of K_{eff} are rather unusual for a dielectric constant. It should be strongly temperature dependent and increase with temperature since p must decrease with temperature. In addition, for heavy trapping (p of the order of 10^6), K_{eff} must be of the order of 10^{-6} or considerably less than the dielectric constant for vacuum. These unusual properties are due to the fact that the electric field "flux lines" originating from the positive metal surface do not all reach the opposite metal but are terminated in the space charge of the insulator. One should not expect to find the capacity of the junction reduced when the capacity is measured by an ac bridge.

Relation (1) may be integrated immediately to give

$$2R+2Qq=U''+U'^2/2, \tag{2}$$

where $2R$ is the first constant of integration.‡ The further change of variable,

$$U=2\ln(y) \tag{3}$$

brings the relation (2) to the form

$$y''-(Qq+R)y=0. \tag{4}$$

For the case $Q=0$, relation (4) can be integrated to

$$y=\cos(wq)+\lambda\sin(wq) \tag{5}$$

where w is the positive square root of $-R$. For $Q\neq 0$, relation (4) can be integrated to

$$y=s^{\frac{1}{3}}[J_{\frac{1}{3}}(s)+\lambda J_{-\frac{1}{3}}(s)] \tag{6}$$

with $s=-(2/3Q)(-Qq-R)^{\frac{3}{2}}$. The quantity, λ, is the second constant of integration. The third constant is taken to be unity since it only serves to fix the absolute value of the potential. The functions $J_{\frac{1}{3}}$ and $J_{-\frac{1}{3}}$ are the Bessel functions of order $\frac{1}{3}$ and $-\frac{1}{3}$ respectively. When w and s are imaginary, it should be understood that the following relations are implied:

$$\cos(iz)=\cosh(z)$$

$$\sin(iz)=i\sinh(z)$$

$$J_p(iz)=\exp(p\pi i/2)I_p(z);\quad(-\pi<\arg z<\pi/2)$$

where I_p is the modified Bessel function.

The Case $Q=0$

Twofold differentiation of U provides the expression for the dimensionless charge density, which can be evaluated at the boundaries to give

$$U_0''=-2w^2(1+\lambda^2) \tag{7}$$

$$U_1''=-2w^2(1+\lambda^2)/(\cos w+\lambda\sin w)^2. \tag{8}$$

Taking the ratio of (7) and (8), member for member, and solving for λ one obtains

$$\lambda=\frac{(U_0''/U_1'')^{\frac{1}{2}}-\cos w}{\sin w}. \tag{9}$$

The positive square root is taken to avoid an infinite potential within the barrier. The potential can then be expressed as

$$U=2\ln\frac{(U_0''/U_1'')^{\frac{1}{2}}\sin wq+\sin w(1-q)}{\sin w} \tag{10}$$

so the contact potential difference is simply

$$\Delta U=\ln(U_0''/U_1'')=\ln[n_c(0)/n_c(L)].$$

The contact potential does not depend upon the amount of trapping. This is a necessary condition which all trapping models must satisfy to be consistent with the general thermodynamic laws. To solve for w one eliminates λ from (7) and (8) and after some algebraic manipulations one finds that

$$\sin^2 w=w^2[(2/-U_0'')+(2/-U_1'')-4(U_0''U_1'')^{-\frac{1}{2}}\cos w] \tag{11}$$

and in the special case where $U_0''=U_1''$ one finds that

$$\cos w/2=w(-U_0''/2)^{-\frac{1}{2}}. \tag{12}$$

The positive square root, $(U_0''U_1'')^{\frac{1}{2}}$, has been taken to correspond to the sign of $(U_0''/U_1'')^{\frac{1}{2}}$ in relation (9).

The electric fields at the boundaries are determined by

$$U_0'=2w\frac{(U_0''/U_1'')^{\frac{1}{2}}-\cos w}{\sin w}$$

$$U_1'=-2w\frac{(U_1''/U_0'')^{\frac{1}{2}}-\cos w}{\sin w}.$$

The solutions for w in (11) and (12) are either real or purely imaginary. If they are real,§ w may be multiple valued. If $w\geq\pi$, then there will be an infinite potential somewhere within the barrier. The restriction $0<w<\pi$ is added on physical grounds so as to make w single valued and avoid the infinite potential.

The Case $Q\neq 0$

If s_0 and s_1 are the values of s at the respective boundaries, then Q and R may be expressed as

$$Q=-(3/2)^2(s_1^{\frac{2}{3}}-s_0^{\frac{2}{3}})^3 \tag{13}$$

$$R=-(3/2)^2(s_1^{\frac{2}{3}}-s_0^{\frac{2}{3}})^2 s_0^{\frac{2}{3}}. \tag{14}$$

Again applying the first two boundary conditions and solving for λ, one has

$$-\lambda=\frac{[J_{1/3}(s_0)-P_0J_{-2/3}(s_0)]}{[J_{-1/3}(s_0)+P_0J_{2/3}(s_0)]}, \tag{15}$$

$$-\lambda=\frac{[J_{1/3}(s_1)-P_1J_{-2/3}(s_1)]}{[J_{-1/3}(s_1)+P_1J_{2/3}(s_1)]}, \tag{16}$$

‡ Relation (2) is a special case of the generalized Ricatti equation with U' as the dependent variable. [For example, see E. L. Ince, *Ordinary Differential Equations* (Dover Publications, New York, 1944).]

§ Solutions to (12) must always be real.

where

$$P_0=[B_0/(1-B_0)]^{\frac{1}{2}}, \quad B_0=9s_0^{\frac{2}{3}}(s_1^{\frac{2}{3}}-s_0^{\frac{2}{3}})^2/-2U_0'';$$
$$P_1=[B_1/(1-B_1)]^{\frac{1}{2}}, \quad B_1=9s_1^{\frac{2}{3}}(s_1^{\frac{2}{3}}-s_0^{\frac{2}{3}})^2/-2U_1''.$$

The sign of P_0 and P_1 is determined by the sign of the electric field at the respective boundaries. For the small Q range the electric fields are essentially the zero current fields and for the large Q range the electric field is essentially the applied field, so the signs may be fixed accordingly.

The elimination of λ from relations (15) and (16) leads to

$$\begin{aligned}&[J_{-1/3}(s_0)J_{1/3}(s_1)-J_{1/3}(s_0)J_{-1/3}(s_1)]\\&\quad-[J_{2/3}(s_0)J_{-2/3}(s_1)-J_{-2/3}(s_0)J_{2/3}(s_1)]P_0P_1\\&\quad+[J_{2/3}(s_0)J_{1/3}(s_1)+J_{-2/3}(s_0)J_{-1/3}(s_1)]P_0\\&\quad-[J_{-1/3}(s_0)J_{-2/3}(s_1)+J_{1/3}(s_0)J_{2/3}(s_1)]P_1=0, \quad (17)\end{aligned}$$

which constitutes the exact solution for the current voltage relation in parametric form. If a value of s_0 is chosen, relation (17) provides the corresponding value of s_1. With this pair of values one determines Q by (13), R by (14), λ by (15) or (16) and ΔU by (3) and (6). Explicit forms for the current voltage relation may be obtained by the use of asymptotic expansions of the Bessel functions. The forms,

$$\begin{aligned}\Delta U&=\frac{4Q^2}{3(-U_1'')^3}[(1-U_1''^2/Q)^{\frac{3}{2}}-1], \quad Q<0\\ \Delta U&=\frac{-4Q^2}{3(-U_0'')^3}[(1+U_0''^2/Q)^{\frac{3}{2}}-1], \quad Q>0\end{aligned} \quad (18)$$

are obtained for the large Q range and are essentially the same as the form obtained by Mott and Gurney for the metal-insulator surface. These forms indicate that, in this range of current, the current-voltage relation is governed by the property of the metal from which electrons are flowing. The other metal acts simply as a sink. The form for small Q is given by

$$\begin{aligned}\Delta U_a=&\,(1/2)\ln(1-Q/w^2)\\&+2\ln[1-(2/-U_0'')^{\frac{1}{2}}(Q/2w^2)(1+2w^2/U_0'')^{\frac{1}{2}}]\\&-\ln\{1-(Q/2w^2)[(2/-U_0'')^{\frac{1}{2}}(1+2w^2/U_0'')^{\frac{1}{2}}\\&\qquad+(2/-U_1'')^{\frac{1}{2}}(1+2w^2/U_1'')^{\frac{1}{2}}]\} \quad (19)\end{aligned}$$

where ΔU_a is the applied potential difference, w is defined by (11) or (12), and the signs of $(1+2w^2/U_0'')^{\frac{1}{2}}$ and $(1+2w^2/U_1'')^{\frac{1}{2}}$ take the signs of the corresponding zero current electric fields. The range of validity is given by $|s_0|$, $|s_1|\gg 1$ for both relations (18) and (19).|| In addition one must require that $|Q/R|\ll 1$ and $|(|R|-|w^2|)/|w^2||\ll 1$ for relation (19).

|| In relation (18) $Q\sim|s_0|^{\frac{4}{3}}$ and $R\sim|s_0|$ when $s_0\rightarrow i\infty$ such that $|s_1-s_0|\rightarrow\infty$. In relation (19) $Q\sim|s_0|^{-1}$ and $R\rightarrow -w^2$ when $s_0\rightarrow\infty$ for real w or when $s_0\rightarrow i\infty$ for imaginary w such that $|s_1-s_0|\rightarrow 0$.

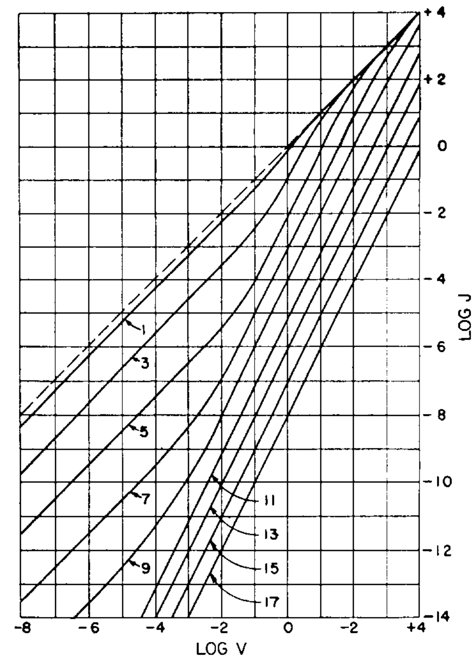

FIG. 1. Current-voltage relation for the special case where $U_0''=U_1''=-1.4\ 10^m$. Curve 1 is for $m=1$; curve 3 is for $m=3$, etc.

DISCUSSION OF RESULTS

The special case where $U_0''=U_1''$ contains one fewer parameter; so, this case will be particularly interesting experimentally even though no rectification can be expected. The calculated current-voltage relation for this case with various values of U_1'' is given in Fig. 1. In order to display the interesting features of this relation on a single graph, the variables,

$$V=\Delta U/2(-U_1'')^{\frac{1}{2}}$$
$$J=-Q/(-U_1'')^{\frac{3}{2}},$$

are employed. For $J\rightarrow\infty$ all curves approach the $V=J$ line asymptotically. For large but decreasing values of J the curves tend toward a slope of two, which is the Child's law analog region for space charge limited current obtained by Shockley and Prim. However, for small U_1'' a slope of two is not reached. In the limit $U_1''\rightarrow 0$, the relation becomes $V=J$ over the entire range. For $J\rightarrow 0$, all curves have a slope of one. The region which must be determined by numerical calculation is the region where the curves are sharply concave upward.

From the current-voltage relation one may determine the resistivity, R_F, as a function of the thickness, L, of the film. For illustration take, along with $U_0''=U_1''$, the reasonable values, $u=300$ cm^2/v sec, $K=5$, $T=300$°K, $F=10^4$ volts/cm applied field. A plot of $\log(R_F/R_\infty)$ against $\log(L/1\text{ cm})$ is given in Fig. 2. The quantity, $R_\infty=1/n_1eu$, is the resistivity at infinite field strength, or the temperature limited resistivity, and is independent of L. Notice that for $pn_c>10^{10}$ cm^{-3} there

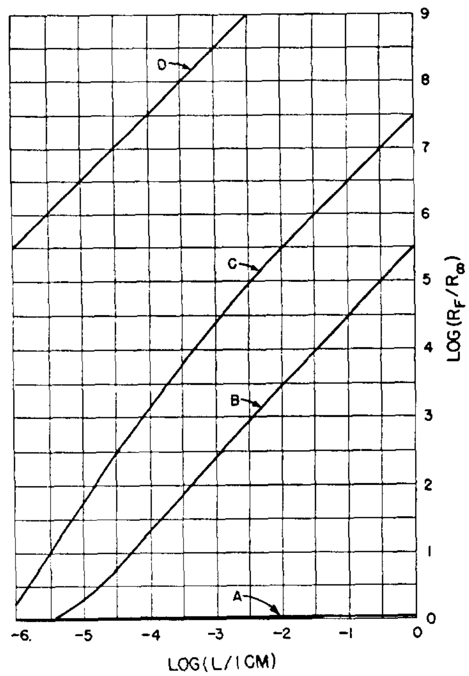

FIG. 2. The ratio of resistivity at constant field to the resistivity at infinitely large field as a function of the thickness of the film bounded by identical metals.

Curve *A* (in the base line) is for $p=1$, $n_c=10^{10}$; curve *B* is for $p=10^6$, $n_c=10^{10}$; curve *C* is for $p=1$, $n_c=10^{18}$; curve *D* is for $p=10^6$, $n_c=10^{18}$. Curves *B*, *C*, and *D* show that even for thick films the resistivity should vary linearly with thickness.

is an unmistakable change in resistivity with thickness, but for $pn_c<10^{10}$ cm^{-3} there is hardly a measurable change. In addition the change in resistivity is most apparent for quite thick films.

It would appear from this analysis that a clear indication for the validity of this model could be obtained experimentally by way of testing for the current-voltage relation and the resistivity as a function of thickness. An attempt was made to verify this model experimentally by preparing the junctions entirely by the vacuum evaporation technique. It was found that in the case of MgF_2 considerable matter transport occurred during the current flow and in the case of amorphous SiO_2 (where matter transport appeared slight) a current noise appeared which gave the appearance of temporary and multiple electronic breakdowns[6] over a rather large range of field strengths. The average dc current increased nonlinearly with the applied potential as one might expect from the model so that an investigator might be misled into feeling that he had a true test of the junction if he employed only the relatively long-response time meter movements rather than a cathode ray oscilloscope presentation of the instantaneous current. Klärmann and Mühlenpfordt[7] tested a Ag-SiO_2-Ag junction made by the vacuum evaporation technique. A similar nonlinear increase of current with applied potential was observed but apparently no investigation of the nature of the instantaneous current was made.

Thin evaporated films have been used in these tests mainly because they may be prepared fresh in the vacuum. One may hope to avoid adsorbed material, which may produce serious surface trapping. However, evaporated films are rarely well-ordered crystals and some materials (NaCl and NaF for example) never form a compact film. The use of thick films prepared by other means is presently limited by the technical difficulty of complete cleaning of adsorbed material. High-energy ion bombardment of self-supporting films such as Al_2O_3, SiO, mica, and numerous organic films should produce a basis for a more nearly ideal junction.

SUMMARY

The effect of the trapping model on the dc current-voltage relation of the metal-insulator-metal junction was the same as if the dielectric constant of the insulator were reduced by a factor $1/p$.

The exact current-voltage relation was obtained in parametric form and was computed for the case of identical metals on the boundaries. For the low current range an almost linear relation was found. Higher currents followed a square-law relation for high values of space charge. Still higher currents followed a linear relation. When space charge effects were negligible, a linear relation was followed for all values of current. The apparent resistivity of the insulator film was computed as a function of its thickness at constant field strength, using reasonable values for the properties of the insulator. It was found that the resistivity should decrease nearly linearly with thickness for thick insulators when boundary charge densities exceeded 10^{10} per cm^3.

Test junctions were prepared entirely by the vacuum evaporation method, but the insulating films were not compact, or exhibited matter transport with the application of an electric field. A more suitable test junction might be prepared using self-supporting insulator films cleaned by ion bombardment.

ACKNOWLEDGMENT

The author wishes to acknowledge the valuable assistance of Dr. E. Katz in this investigation.

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