NASA Technical Memorandum 87262

A Computer Program to Calculate the Resistivity of a Thin Film Deposited on a Conductive Substrate From Four-Point Probe Measurements

(NASA-TM-87262) A COMPUTER PROGRAM TO CALCULATE THE RESISTIVITY OF A THIN FILM DEPOSITED ON A CONDUCTIVE SUBSTRATE FROM FOUR-POINT PROBE MEASUREMENTS (NASA) 28 p HC A03/MF A01 CSCL 09B G3/61

N86-22150

Unclas 0584[illegible]

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March 1986

NASA

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SUMMARY

This paper deals with the use of the four-point probe to measure the resistivity of a thin film of conducting material deposited on another layer of conducting material. Such measurements occur, for instance, in silicon carbide (SiC) research, where it is necessary to grow the SiC on a silicon (Si) substrate. The presence of the silicon substrate will introduce errors in the measured resistivity of the SiC.

Starting from basic principles, and expression for the ratio of measured voltage difference to injected current [$\Delta V/I$] is developed. This expression involves the probe spacing, relative thicknesses of the layers, and the substrate resistivity as parameters, as well as the unknown resistivity of the deposited layer. The unknown resistivity can be found by iteratively evaluating the theoretical expression. This must be done numerically. A full description of the numerical techniques involved, and the computer programs used, is given.

Finally a comparison with previously published results is presented, together with a detailed description of how to use the programs to find resistivities, as well as plot curves displaying the change in $\Delta V/I$ as a function of the thicknesses of the layers, and their resistivities.

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INTRODUCTION

One of the ways in which a semiconductor material is characterized is by the measurement of its resistivity. In the development of silicon carbide for use as semiconductor material for high temperature applications, it became necessary to measure the resistivity of the thin film while it still was attached to the silicon upon which it had been grown epitaxially. A method of calculating the "true" resistivity of a deposited layer on a substrate of finite and different resistivity was discussed by Brown and Jakeman (ref. 1). The theory was presented in a cursory fashion, and no mention was made of a technique (i.e., and analysis, or series of programs) to determine the resistivity, or conductivity. Our intent is to remedy this defect with a presentation of the theory in depth, and a library of programs which calculate the correction factors necessary for evaluation of the equation presented by Brown.

The situation is as shown in figure 1. Current of magnitude I is injected at probe A and withdrawn at probe B, and the voltage difference, ΔV, between probes 1 and 2 is measured. The subject of this paper is the determination of the unknown conductivity, σ_1, or resistivity, ρ_1, of the thin film in terms of the known quantitites $\Delta V/I$, ω_1, ω_2 (the thicknesses of the respective layers), and σ_2 (the conductivity of the substrate).

THEORY

Governing Equations and Boundary Conditions

It is assumed that the materials obey Ohm's Law, i.e.,

$$\vec{J} = \sigma\vec{E} \tag{1}$$

where $\vec{J}$ is the current density in A/m^2, σ is the conductivity $(\Omega\text{-m})^{-1}$, and $\vec{E}$ is the electric field in V/m.

The current density $\vec{J}$ satisfies the continuity equation for the electric charge in the form

$$\vec{\nabla} \cdot \vec{J} + \frac{\partial\varphi}{\partial t} = 0 \tag{2}$$

where φ is the electric charge density, in C/m^3. For steady currents, there is no accumulation of charge at any point, so $\partial\varphi/\partial t$ is zero, and

$$\vec{\nabla} \cdot \vec{J} = 0 \tag{3}$$

From equation (1)

$$\vec{\nabla} \cdot (\sigma\vec{E}) = 0 \tag{4}$$

The electric field $\vec{E}$ is derivable from a potential function V, since $\vec{\nabla} \times \vec{E} = 0$,

$$\vec{E} = -\vec{\nabla}V \tag{5}$$

Combining equations (4) and (5),

$$\vec{\nabla} \cdot (\sigma\vec{\nabla}V) = 0$$

or if σ is constant,

$$\vec{\nabla}^2 V = 0 \tag{6}$$

Thus the potential V satisfies Laplace's equations inside the two layers. The boundary conditions satisfied by V may be found by analogy with electrostatics. For a charge-free region, Gauss's law (ref. 2) is given by

$$\vec{\nabla} \cdot (\epsilon\vec{E}) = 0 \tag{7}$$

where ϵ is the permittivity. Comparing equation (7) with equation (4), it is seen that σ in the steady current problem plays the role of ϵ in the electrostatic case. Equation (7) leads to the boundary condition (ref. 3).

$$V_1 = V_2, \quad \epsilon_1 \frac{\partial V_1}{\partial n} = \epsilon_2 \frac{\partial V_2}{\partial n}$$

where $\partial/\partial n$ indicates the normal derivative at the boundary. Replacing ε by σ, our boundary conditions become

$$V_1 = V_2, \quad \sigma_1 \frac{\partial V_1}{\partial n} = \sigma_2 \frac{\partial V_2}{\partial n} \tag{8}$$

Equations (6) and (8), together with the field about a point current source (from appendix B), are sufficient to find the function V.

Solution of Equations

The method of attack is to find the potential due to a single point current source and then use superposition to find the potentials due to the two sources at A and B.

The $z = 0$ plane is at the top of the upper plane in figure 1, and the positive z axis extends into the material. The two planes are bounded at $z = 0$, $z = \omega_1$, and $z = \omega_1 + \omega_2$. Since we are considering only the source at A for the time being, the problem has azimuthal symmetry; that is, the potential has no angular dependence about the z-axis. It is therefore convenient to use cylindrical coordinates.

In cylindrical coordinates, Laplace's equation $\vec{\nabla}^2 V = 0$, assumes the form

$$\frac{1}{r}\frac{\partial}{\partial r}\left[r\frac{\partial V}{\partial r}\right] + \frac{1}{r^2}\frac{\partial^2 V}{\partial \theta^2} + \frac{\partial^2 V}{\partial z^2} = 0 \tag{9}$$

where r is the distance from the z-axis and θ is the angular displacement. Equation (9) may be solved by separation of variables; that is $V(r,\theta,z)$ is written as

$$V(r,\theta,z) = R(r)\,\Theta(\theta)\,Z(z) \tag{10}$$

in which case equation (9) assumes the form

$$\frac{1}{rR}\left[r\frac{dR}{dr}\right] + \frac{1}{r^2\Theta}\frac{d^2\Theta}{d\theta^2} = -\frac{1}{Z}\frac{d^2 Z}{dz^2} \tag{11}$$

The left side of equation (11) is a function of r and θ, and the right side is a function of z only. In order for equation (11) to be true for all values of $r \geq 0$, $-\pi \leq \theta < \pi$, $-\infty \leq z \leq \infty$, both sides must equal a constant. Hence equation (11) is written

$$\frac{1}{rR}\frac{d}{dr}\left[r\frac{dR}{dr}\right] + \frac{1}{r^2\Theta}\frac{d^2\Theta}{d\theta^2} = -\frac{1}{Z}\frac{d^2 Z}{dz^2} = -k^2$$

Therefore Z satisfies the equation

$$\frac{d^2 Z}{dz^2} = k^2 Z$$

which has the solution

$$Z = E_k e^{kz} + F_k e^{-kz} \tag{12}$$

The solution for Θ is found in a similar fashion. Moving the k^2 to the left side and multiplying by r^2, equation (11) becomes

$$\frac{r}{R}\frac{d}{dr}\left[r\frac{dR}{dr}\right] + k^2r^2 = -\frac{1}{\Theta}\frac{d^2\Theta}{d\theta^2} = n^2 \tag{13}$$

so that Θ satisfies the equation

$$\frac{d^2\Theta}{d\theta^2} = -n^2\Theta$$

If the potential is to be single valued in θ, n must be an integer, and

$$\Theta(\theta) = C_n \cos(n\theta) + D_n \sin(n\theta) \tag{14}$$

The above choice of separation constants leads to solutions which are periodic in θ and can be made to vanish at $z = \pm\infty$.

This leaves only the equation for $R(r)$. Multiplying by R, equation (13) can be rewritten as

$$r\frac{d}{dr}\left[r\frac{dR}{dr}\right] + \left[k^2r^2 - n^2\right]R = 0 \tag{15}$$

This is Bessel's differential equation, and R is written

$$R(r) = A_n J_n(kr) + B_n Y_n(kr) \tag{16}$$

where J_n and Y_n are the Bessel functions of order n of the first and second kind. Both are oscillatory functions which vanish are $r = \infty$, but only J_n is finite at $r = 0$. In our problem, $V(0,\theta,z)$ must be $< \infty$, so Y_n is excluded. Further, since there is no angular dependence, $n = 0$, and our solution is written in terms of $J_0(kr)$.

For problems involving boundary conditions on cylindrical boundaries at finite values of r and no angular dependence, the solution $V(r,z)$ involves a sum over discrete values of k. As an example, if V is to vanish on a cylinder of radius a, the solution inside the cylinder is

$$V(r,z) = \sum_{i=1}^{\infty} A_i e^{-k_i|z|} J_0(k_i r) \tag{17}$$

where $ak_i = x_i$, the i^{th} zero of $J_0(x)$. In this way each term in equation (17) vanishes at $r = a$.

Now, as $a \to \infty$, $k_i = x_i/a$ becomes a continuous variable, and the solution (eq. (17)) becomes

$$V(r,z) = \int_0^\infty f(k) e^{-k|z|} J_o(kr)\, dk \tag{18}$$

This is the form of the solution to be used in finding the potential inside the two conducting layers shown in figure 1, which are assumed to extend radially to infinity. It can be verified that equation (18) satisfies Laplace's equation.

Application to the Four Point Probe

The potential from the point current source at A will be found first; the total potential due to the source at A and sink at B may then be constructed by algebraic addition.

According to appendix B, and the previous discussion, the potential in the top layer due just to the source at point A is

$$V_A = \frac{Q}{\sqrt{r^2 + z^2}} = Q \int_0^\infty e^{-kz} J_o(kr)\, dk \tag{19}$$

where

$$Q = \frac{I}{2\pi\sigma_1} \tag{20}$$

To V_A are then added terms of the form (eq. (18)) due to the currents flowing along the discontinuities at $z = 0$, and $z = \omega_1$. If this were an electrostatics problem, these additional terms would be due to charge distributions at the discontinuities. Combining equations (18) and (19), the potential in the top region is

$$V_1 = \int_0^\infty \left[f_1(k) e^{kz} + g_1(k) e^{-kz} \right] J_o(kr)\, dk + \frac{Q}{\sqrt{r^2 + z^2}} \tag{21}$$

$$= \int_0^\infty \left[f_1(k) e^{kz} + g_1(k) e^{-kz} + Q e^{-kz} \right] J_o(kr)\, dk \tag{22}$$

Likewise, in the bottom layer the potential is

$$V_2 = \int_0^\infty \left[f_2(k) e^{kz} + g_2(k) e^{-kz} \right] J_o(kr)\, dk \tag{23}$$

Once the functions f_1, f_2, g_1, and g_2 are determined, the potential every where inside the two layers will be known, although, since we need only the potential at $z = 0$, only f_1 and g_1 are needed.

At $z = 0$, the first of the boundary conditions, equation (8), reduces to

$$\frac{\partial V_1}{\partial z}(r,0) = 0 \tag{24}$$

since in the region $z < 0$, $\sigma = 0$. At $z = \omega_1$, equation (8) gives

$$V_1(r,\omega_1) = V_2(r,\omega_1) \tag{25}$$

$$\sigma_1 \frac{\partial V_1(r,\omega_1)}{\partial z} = \sigma_2 \frac{\partial V_2(r,\omega_1)}{\partial z} \tag{26}$$

The conductivity for $z > \omega_1 + \omega_2$ is zero, so again

$$\frac{\partial V_2(r,\omega_1 + \omega_2)}{\partial z} = 0 \tag{27}$$

The four conditions (24) to (27) are sufficient to determine the four unknown functions f_1, g_1, f_2, and g_2, which appear in equations (21) to (23).

Applying equation (24) to (21),

$$\frac{\partial V_1}{\partial z} = \int_0^\infty k\left[f_1 e^{kz} - g_1 e^{-kz}\right] J_0(kr)\, dk - \frac{Qz}{(r^2 + z^2)^{3/2}}$$

and, at $z = 0$,

$$\frac{\partial V_1(r,0)}{\partial z} = \int_0^\infty k\left[f_1(k) - g_1(k)\right] J_0(kr)\, dk = 0 \tag{28}$$

Since equation (28) must be true for all $r > 0$,

$$f_1(k) - g_1(k) = 0 \tag{29}$$

Note that equation (22) was not used in setting $\partial V_1(r,0)/\partial z = 0$ since

$\int_0^\infty e^{-kz} J_0(kr)\, dk$ is not differentiable at $z = 0$.

The next two boundary conditions (25) and (26) give, respectively

$$\int_0^\infty \left[f_1 e^{k\omega_1} + g_1 e^{-k\omega_1} + Qe^{-k\omega_1}\right] J_o(kr)\, dk$$

$$= \int_0^\infty \left[f_2 e^{k\omega_1} + g_2 e^{-k\omega_1}\right] J_o(kr)\, dk$$

and

$$\sigma_1 \int_0^\infty k \left[f_1 e^{k\omega_1} - g_1 e^{-k\omega_1} - Qe^{-k\omega_1}\right] J_o(kr)\, dk$$

$$= \sigma_2 \int_0^\infty k \left[f_2 e^{k\omega_1} - g_2 e^{-k\omega_1}\right] J_o(kr)\, dk$$

Again, since these equations are to be true for all r, the integrands must be equal, whence

$$f_1 e^{k\omega_1} + g_1 e^{-k\omega_1} - f_2 e^{k\omega_1} - g_2 e^{-k\omega_1} = -Qe^{-k\omega_1} \tag{30}$$

and

$$\sigma_1 f_1 e^{k\omega_1} - \sigma_1 g_1 e^{-k\omega_1} - \sigma_2 f_2 e^{k\omega_1} + \sigma_2 g_2 e^{-k\omega_1} = \sigma_1 Q\left(e^{-k\omega_1}\right) \tag{31}$$

Finally, applying equations (23) and (27),

$$f_2 e^{k(\omega_1+\omega_2)} - g_2 e^{-k(\omega_1+\omega_2)} = 0 \tag{32}$$

Rewriting equation (32) as

$$f_2 e^{k\omega_1} = e^{-2k\omega_2}\left[g_2 e^{-k\omega_1}\right]$$

equations (30) and (31) become, after substitution,

$$f_1 e^{k\omega_1} + g_1 e^{-k\omega_1} - g_2 e^{-k\omega_1}\left[1 + e^{-2k\omega_2}\right] = -Qe^{-k\omega_1} \tag{33}$$

and

$$\sigma_1 f_1 e^{k\omega_1} - \sigma_1 g_1 e^{k\omega_1} + \sigma_2 g_2 e^{-k\omega_1}\left[1 - e^{2k\omega_2}\right] = \sigma_1 Q e^{k\omega_1} \tag{34}$$

Eliminating g_2 between equations (33) and (34),

$$f_1 e^{k\omega_1}\left[\sigma_1\left(1 + e^{-2k\omega_2}\right) + \sigma_2\left(1 - e^{-2k\omega_2}\right)\right]$$

$$- g_1 e^{-k\omega_1}\left[\sigma_1\left(1 + e^{-2k\omega_2}\right) - \sigma_2\left(1 - e^{-2k\omega_2}\right)\right]$$

$$= Q e^{-k\omega_1}\left[\sigma_1\left(1 + e^{-2k\omega_2}\right) - \sigma_2\left(1 - e^{-2k\omega_2}\right)\right]$$

Upon rearrangement, this becomes

$$f_1 e^{k\omega_1}\left[(\sigma_1 + \sigma_2) + (\sigma_1 - \sigma_2)e^{-2k\omega_2}\right] - g_1 e^{-k\omega_1}\left[(\sigma_1 - \sigma_2) + (\sigma_1 + \sigma_2)e^{-2k\omega_2}\right]$$

$$= Q e^{-k\omega_1}\left[(\sigma_1 - \sigma_2) + (\sigma_1 + \sigma_2)e^{-2k\omega_2}\right]$$

Finally, making use of equation (29) (that $f_1 = g_1$), multiplying through by $e^{k\omega_1}$, and dividing through by the quantity $(\sigma_1 + \sigma_2)$,

$$f_1(k) = \frac{Q\left(R + e^{2k\omega_2}\right)}{e^{2k\omega_1}\left[1 + Re^{-2k\omega_2}\right] - \left[R + e^{-2k\omega_2}\right]}$$

or

$$f_1(k) = \frac{Q}{e^{2ks\omega_1/s}\left[\dfrac{1 + Re^{-2ks\omega_2/s}}{R + e^{-2ks\omega_2/s}}\right] - 1} = Qf(ks) \tag{35}$$

where we have made use of the definition

$$R = \frac{\sigma_1 - \sigma_2}{\sigma_1 + \sigma_2} = \frac{\rho_2 - \rho_1}{\rho_2 + \rho_1} \tag{36}$$

The quantities $\rho_1 = 1/\sigma_1$, and $\rho_2 = 1/\sigma_2$ are the resistivities.

We are interested in the potential difference between the two probes at points 1 and 2 in figure 1, when a current I is injected at point A and withdrawn at point B. From equations (21) and (29), the potential on the plane $z = 0$ due to the current entering at A is

$$V(r,0) = \frac{Q}{r} + 2Q \int_0^{\infty} f(ks)J_o(kr)\, dk$$

Since the potentials add algebraically, the potential at point 1 due to source Q_A at point A, and a source Q_B at point B, separated from point A by the distance is

$$V_{p_1} = \frac{Q_A}{s} + 2Q_A \int_0^{\infty} f(ks)J_o(ks)\, dk + \frac{Q_B}{2s} + Q_B \int_0^{\infty} f(ks)J_o(2ks)\, dk \qquad (37)$$

Likewise, the potential at point 2, due to the same sources, is

$$V_{p_2} = \frac{Q_A}{2s} + 2Q_A \int_0^{\infty} f(ks)J_o(2ks)\, dk + \frac{Q_B}{s} + 2Q_B \int_0^{\infty} f(ks)J_o(ks)\, dk \qquad (38)$$

The measured quantity is the voltage difference between points 1 and 2

$$\Delta V = V_{p_1} - V_{p_2} = \frac{Q_A - Q_B}{2s} + 2(Q_A - Q_B) \int_0^{\infty} f(ks) \left[J_o(ks) - J_o(2ks)\right] dk$$

In our case, the sources are equal and opposite in sign ($Q_A = - Q_B = Q$), and

$$\Delta V = \frac{Q}{s} + 4Q \int_0^{\infty} f(ks) \left[J_o(ks) - J_o(2ks)\right] dk \qquad (39)$$

Making the change of variable ($t = ks$) and defining the dimensionless quantities

$$\lambda = \frac{s}{2\omega_1}; \quad W = \frac{\omega_2}{\omega_1} \qquad (40)$$

equation (39) becomes, after using the definition of Q found in equation (20)

$$\frac{\Delta V}{I} = \frac{1}{2\pi s \sigma_1} \left[1 + 4 \int_0^{\infty} g\left[\frac{t}{\lambda}\right] \left[J_o(t) - J_o(2t)\right] dt \right] \qquad (41)$$

with the symbolism

$$g(x) = \cfrac{1}{e^{x}\left[\cfrac{1 + Re^{(Wx)}}{R + e^{-(Wx)}}\right] - 1} \tag{42}$$

The difference $J_0(t) - J_0(2t)$ which appears in equation (41) may be evaluated using an integral representation for $J_0(t)$ (ref. 4).

$$J_0(t) = \frac{1}{\pi}\int_0^{\pi} \cos\left[t \sin(\theta)\right] d\theta \tag{43}$$

whence

$$J_0(t) - J_0(2t) = \frac{1}{\pi}\int_0^{\pi} \left[\cos\left[t \sin(\theta)\right] - \cos\left[2t \sin(\theta)\right]\right] \theta \tag{44}$$

Using the identity

$$\cos(\alpha) - \cos(\beta) = 2 \sin\left[\frac{\alpha + \beta}{2}\right] \sin\left[\frac{\beta - \alpha}{2}\right]$$

equation (44) becomes

$$J_0(t) - J_0(2t) = \frac{2}{\pi}\int_0^{\pi} \left[\sin\left[\frac{3}{2}t \sin(\theta)\right] \sin\left[\frac{1}{2}t \sin(\theta)\right]\right] d\theta \tag{45}$$

and equation (41) becomes

$$\frac{\Delta V}{I} = \frac{1}{2\pi\sigma_1 S}\left[1 + \frac{8}{\pi}\int_0^{\infty} g\left[\frac{t}{\lambda}\right]\int_0^{\pi} \sin\left[\frac{3}{2}t \sin(\theta)\right] \sin\left[\frac{1}{2}t \sin(\theta)\right] d\theta\, dt\right]$$

where $g(x)$ is defined as in equation (42). The double integral, equation (46), is the basis for the programs described in appendix C; the details of which are found in the next section.

PROGRAMMING

Solution for the Double Integral

The integral of equation (46) cannot be evaluated analytically. However, Gaussian quadrature (ref. 5) provides a fast, accurate method of evaluating the double integral numerically. In an "m" point Gaussian quadrature, the integrand is evaluated at points determined by the roots of an m^{th} order Legendre polynomial, and summed, with predetermined weighting factors, to provide an approximation to the integral over the range of integration. For the purposes of our program it was decided that a 6 point quadrature would yield sufficient accuracy.

Before the integral over t can be evaluated, the integral over θ must be performed. Therefore, we rewrite equation (46) as

$$\frac{\Delta V}{I} = \frac{\rho_1}{2\pi s}\left[1 + 4\int_0^{\infty} g\left[\frac{t}{\lambda}\right] K_1(t)\, dt\right] \tag{47}$$

where, using equation (45)

$$K_1(t) = J_0(t) - J_0(2t)$$

or

$$K_1(t) = \frac{2}{\pi}\int_0^{\pi} \sin\left[\frac{3}{2}t\,\sin(\theta)\right]\,\sin\left[\frac{1}{2}t\,\sin(\theta)\right]\, d\theta \tag{48}$$

Because of the change of variable in equation (41), $K_1(t)$ is a function of t only, and is evaluated at the same points, regardless of the value of s, ρ_1, ρ_2, ω_1, or ω_2. The points at which $K_1(t)$ is evaluated are determined by the zeroes of the integrand of equation (47). Two factors influence the evaluation of this integral. First, an integral with upper limit of ∞ is difficult to integrate numerically because the algorithm to be used requires the upper limit be specified. Second, Gaussian quadrature yields more accurate results if the integration is performed over subintervals determined by the zeros of the integrand. Both factors are taken into account with the decision to integrate between the zeroes of the integrand, and to sum these results until the change in the total is negligible.

The problem of solving equation (46) is then divided into three parts: finding the zeroes of the integrand

$$K_2(t) = g\left[\frac{t}{\lambda}\right] K_1(t) \tag{49}$$

evaluating

$$P_j = \sum_{i=0}^{j}\int_{Z_i}^{Z_{i+1}} K_2\, dt \tag{50}$$

and finally, solving

$$\frac{\Delta V}{I} = \frac{\rho_1}{2\pi s}\left[1 + 4P_j\right] \tag{51}$$

for ρ_1, where P_j is found by increasing j until $|P_j - P_{j+1}|$ is less than the resolution of the computer.

The variable $g[t/\lambda]$, as given by equation (42), is a monotonically decreasing function of t, and has only the one zero (at $t = \infty$). Therefore, the zeroes of K_2 are identical to the zeroes of K_1. The first programming step, then, is to determine the zeroes of $K_1(t)$. The number of zeroes of $K_1(t)$ is determined by the relative [illegible]es of the other parameters. We found that for all cases attempted, 50 zeroes was sufficient to accurately evaluate the integral. Because equation (48) is a function of t only, the zeroes of the integrand are constant, and can be found once and stored in a file. With the zeroes of the integrand known, the points at which $K_1(t)$ is evaluated are known, and the value of $K_1(t)$ at these points can be found, and stored in a file.

The order of programming is thus:

		PROGRAM
1.	Determine first "j" zeroes of $K_1(t)$	ZERO
2.	Determine values of $K_1(t)$ at evaluation points	BESCAL
3.	Plot $\Delta V/I$ versus ρ_2/ρ_1 for various s, ω_1, ω_2. and ρ_2	FPPPLT
4.	Determine ρ_1 for given $\Delta V/I$, ρ_2, ω_1, ω_2, and s	FOUR

The listings for these programs, written in FORTRAN-77 (ref. 6) for an IBM-PC, can be obtained by contacting COSMIC (The Computer Software Management and Information Center [LEW No. 14389]). An explanation of the procedure required for running these programs is found in appendix C.

Program Explanation

The first two programs, ZERO and BESCAL use the subroutine BESDIF to evaluate equation (48), at a given value of t. BESDIF uses the 6 point Gaussian quadrature over 30 subintervals spanning the range from 0 to π. ZERO uses an interval halving technique to find the first "j" zeroes of the difference, $J_0(t) - J_0(2t)$ (with "j" arbitrarily recommended to be 50). The first zero is known to occur at $t = 0$. The program stores this initial value in the ASCII file ZERO.DAT, and begins the algorithm to identify the rest of the zeroes. Starting at $t = 1$, with an interval of 1, ZERO calculates $K_1(t)$ until the result changes sign At that point the interval is [illegible]lved, the direction of increment is reversed, and the program calculates values of $K_1(t)$ until the sign changes again. This process repeats until the desired accuracy (a recommended 5 digits) is achieved. When the zero is found sufficiently accurately, the value of t which produced the zero is stored, the interval is reset to 1, and the program repeats until the desired number of zeroes is found.

The program BESCAL, using the location of these zeroes, then calculates the values of $K_1(t)$ necessary for the other two programs to evaluate the integral of equation (46). For each interval between zeroes, BESCAL calculates and stores the values of $K_1(t)$ in the file TWOBES.DAT.

With the locations of the zeroes known, and the values of $K_1(t)$ known at the points of evaluation, the two main programs, FPPPLT and FOUR can be executed. FPPPLT calculates an array of numbers suitable for plotting. The plots appearing in this report were generated using an off-the-shelf spread sheet program (ref. 7). The plots produced are $\log(\Delta V/I)$ versus $\log(\rho_2/\rho_1)$ for constant W, s and ρ_2, and for various values of λ. This program was used by the authors primarily as a check of the algorithms used.

FOUR, the more useful of the two programs, calculates a ρ_1 to correspond to a given ω_1, ω_2, ρ_2, s, and $\Delta V/I$. This is accomplished by multiplying both sides of equation (47) by $2\pi s/\rho_2$

$$\left[\frac{\Delta V}{I}\right] \frac{2\pi s}{\rho_2} = \frac{\rho_1}{\rho_2}\left[1 + 4\int_0^{\infty} g\left[\frac{t}{\lambda}\right] \cdot K_1(t)\ dt\right] \tag{52}$$

The left side of equation (52) can be evaluated from experimentally determined parameters. The right side of equation (52) is calculated from an initial guess of ρ_1, keeping in mind that g(x) is a function of ρ_1, as given by equations (42) and (36). Theoretically the right side of equation (52) can be re-evaluated repeatedly until the equality is achieved. In practice the intermediate functions F' and F are calculated as:

$$F' = \left[\frac{\Delta V}{I}\right] \frac{2\pi s}{\rho_2} \tag{53}$$

and

$$F = \frac{\rho_1}{\rho_2}\left[1 + 4\int_0^{\infty} g\left[\frac{t}{\lambda}\right] \cdot K_1(t)\ dt\right] \tag{54}$$

if $|F' - F|$ is less than the required tolerance, then the value of ρ_1 used is displayed as the "correct" resistivity. Otherwise, the guess for ρ_1 is modified according to the sign of the quantity $F' - F$, and if necessary, the interval is halved, until the error is less than the required tolerance. Because most of the "number crunching" needs be performed once for all possible values of the variables, the calculation speed of the algorithm is very high.

RESULTS

The curves of figure 2 were produced using data generated by the program FPPPLT. The parameters were chosen to correspond to the parameters chosen by Brown (ref. 1), in order to compare figure 2 with Brown's results. The shapes of the curves are identical to those produced by Brown. The difference in the plots is that the graphs of this paper are of $\Delta V/I$ versus ρ_2/ρ_1, and in Brown's report, the plots are of the function F (identical to F in this paper) versus σ_1/σ_2. The abscissa is the same in both cases, but the ordinate in Brown's paper does not correspond to a measurable quantity. Since F' is a function of the probe spacing, and the resistivity of the substrate, these two parameters were set to one in figures 2(a) to (c). With this choice of parameters,

$$F = \frac{\Delta V}{I}(2\pi) \tag{55}$$

Taking this into account, the plots of this paper are identical with Brown's plots.

Figure 3 shows the variation of $\Delta V/I$ as a function of the ratio of the resistivities of the layers as well as a function of the thickness of the deposited layer. When the resistivities are approximately equal ($\rho_2/\rho_1 \cong 1$), $\Delta V/I$ is a function of the thickness of the deposited layer only in the sense that $\Delta V/I$ is dependent on the thickness of the sum of the two layers $(\omega_1 + \omega_2)$. Intuitively, this can be seen to be correct, for if the resistivities are equal, the division between the materials disappears, and the measurement of $\Delta V/I$ is that of a single layer. Since the deposited layer varies from less than 2 percent to less than 10 percent of the total thickness, the variation in $\Delta V/I$ is relatively small. As the ratio ρ_2/ρ_1 increases, the thickness of the deposited layer comes more into play. In general, it can be seen that the thicker the deposited layer, the lower the measured value of $\Delta V/I$. In addition, the slope of the curve steepens as the ratio ρ_2/ρ_1 increases. This implies that the algorithm is more accurate for values of $\rho_1 << \rho_2$.

In order to verify the algorithm in the program FOUR, the two examples from Brown's paper were chosen to be used in our calculation. Table I reproduces the applicable numbers from Brown's table II, augmented by the results obtained using the program FOUR.

The results of our program agree closely with the results published by Brown, and with the known values for the substances in question. The slight discrepancies are caused by the increased resolution of our machine, and by assumed roundoff errors associated with the numbers published by Brown. Without knowing the algorithm used by Brown, it is difficult to make judgments about his techniques. However, it must be noted that advances in computer technology, in the 20 years since Brown reported his results, have made the evaluation of these equations much easier, and more accurate than before. In addition to this is the fact that the program FOUR solves the equation for ρ, and Brown's results are given in terms of $1/\rho = \sigma$.

CONCLUSIONS

As can be seen from the plots, and from the numbers generated to produce table 1, the algorithm devised solves the problem as well as the unknown algorithm designed by Brown. Along with a detailed explanation of the software generated in this effort, we tried to explain the process of arriving at the integral presented by Brown, starting from the governing equation, and boundary conditions. It is hoped that the details in the solution are sufficient to enable the reader to use these results in the solution of the class of problems where resistivity measurements are needed for a substance deposited on a substrate of higher resistivity than the deposited layer.

APPENDIX A

NOMENCLATURE

A	probe at which current is injected
A_n	coefficient of 1st independent solution to Bessel's equation, V
B	probe at which current is withdrawn
B_n	coefficient of 2nd independent solution to Bessel's equation, V
C_n	coefficient of 1st independent solution for $\Theta(\theta)$
c	constant to be determined in solving for potential due to an isolated point source
D_n	coefficient of 2nd independent solution for $\Theta(\theta)$
$\vec{E}$	electric field, V/m
E_k	coefficient of 1st independent solution for $Z(z)$
F	intermediate function used in computing resistivity
F'	intermediate function calculated from measured parameters
F_k	coefficient of 2nd independent solution for $Z(z)$
f	function to be determined in solving the potential problem in the continuous case
f_1	function solved in the deposited layer due to current input at point A
f_2	function solved in the substrate due to current input at point A
g	function f redefined in terms of x rather than ks
g_1	function (akin to f_1) in the deposited layer due to current withdrawn at B
g_2	function (akin to f_2) in the substrate due to current withdrawn at B
I	current injected at probe A, A
$\vec{J}$	current density, A/m^2
J_n	Bessel function of the first kind of order n
J_0	Bessel function of the first kind of order 0
j	number of zeroes of $K_1(t)$ to be found

K_1	difference $J_0(t) - J_0(2t)$
K_2	$g(t/\lambda)\ K_1(t)$
k	separation constant, m^{-1}
m	order of Legendre polynomial used in Gaussian quadrature
n	separation constant, m^{-1}
P_m	value of $\Sigma_m \int K_2\ dt$ using "m" zeroes
Q	Psuedo charge (analogous to charge in electrostatics) $Q = I/(2\pi\sigma_1)$, V/m
Q_A	Psuedo charge at point A, V/m
Q_B	Psuedo charge at point B, V/m
R	resistivity variable $(\rho_2 - \rho_1)/(\rho_2 + \rho_1)$
$R(r)$	potential function in the r direction, V
r	radial coordinate
$\hat{r}$	unit vector in r direction
s	spacing between any two adjacent probes in four point apparatus, m
$\vec{s}$	elemental area on surface of sphere
$V(r,\theta,z)$	potential function, V
V_A	potential function at probe A, V
V_{p_1}	potential function at point 1, V
V_{p_2}	potential function at point 2, V
V_1	potential function in deposited layer, V
V_2	potential function in substrate, V
W	ratio of substrate thickness to thickness of deposited layer
Y_n	Bessel function of the second kind of order n
$Z(z)$	potential function in the z direction
z	axial coordinate
$\|z\|$	absolute value of z

ΔV	voltage difference between probes 1 and 2, V
ϵ	permittivity, F/m
ϵ_1	permittivity of first layer, F/m
ϵ_2	permittivity of second layer, F/m
$\Theta(\theta)$	potential function in the θ direction
θ	angular coordinate
λ	twice the ratio of probe spacing to deposited layer thickness
ρ	resistivity, Ω-m
ρ_1	resistivity in the deposited layer, Ω-m
ρ_2	resistivity in the substrate, Ω m
σ	conductivity, $(\Omega\ m)^{-1}$, $\Omega^{-1}m^{-1}$
σ_1	conductivity of the deposited layer, $\Omega^{-1}m^{-1}$
σ_2	conductivity of the substrate, $\Omega^{-1}m^{-1}$
φ	electric charge density, C/m^3
ω_1	thickness of the deposited layer, m
ω_2	thickness of the substrate, m
∂	partial derivative operator
$\vec{\nabla}$	vector differential operator
$\vec{\nabla}^2$	Laplacian operator

APPENDIX B

The Electric Potential due to an Isolated Point Current Source

Consider a point current source of output I located at an origin within a medium of uniform conductivity, σ. By symmetry, the current density vector, J must vary as $1/r^2$, where r is the distance from the source, since the total current passing through any sphere surrounding the source is I, and the area of the sphere is proportional to r^2. That is

$$\oint_{\text{sphere}} \vec{J} \cdot \vec{ds} = I \tag{B.1}$$

where $\vec{ds}$ is the element of area on the surface of the sphere,

$$\vec{ds} = \hat{r}\, r^2 \sin\theta \, d\theta \, d\varphi \tag{B.2}$$

Since $\vec{J} = \sigma\vec{E}$, the electric field $\vec{E}$ is also directed along $\hat{r}$ and is proportional to $1/r^2$. Thus

$$\vec{E} = \frac{c}{r^2}\hat{r} \tag{B.3}$$

The unknown constant, c, in equation (B.3) can be determined from equations (B.1) and (B.2):

$$\oint_{\text{sphere}} \vec{J} \cdot \vec{ds} = \sigma \int_0^{2\pi} \int_0^{\pi} \left[\frac{c}{r^2}\hat{r}\right] \cdot \left[\hat{r}\, r^2 \sin\theta \, d\theta \, d\varphi\right]$$

$$= \sigma c \int_0^{2\pi} \int_0^{\pi} \sin\theta \, d\theta \, d\varphi = 4\pi\sigma c = I \tag{B.4}$$

or

$$c = \frac{I}{4\pi\sigma} \tag{B.5}$$

Then, from equation (B.3), the electric field becomes:

$$\vec{E} = \frac{I}{4\pi\sigma}\frac{\hat{r}}{r^2} \tag{B.6}$$

This is the electric field about an isolated current source of strength I. Since the potential, V, is related to $\vec{E}$ by $\vec{E} = -\nabla V$, the potential (referenced to zero at infinity) is:

$$V = \frac{I}{4\pi\sigma r} \tag{B.7}$$

The electric field, as given by equation (B.6), and the corresponding potential, from equation (B.7), apply to the case of an isolated point source from which the current density is independent of direction. In our case, however, the current (in cross section) is confined to the upper half plane ($\sigma = 0$ for $z < 0$). Then the limits on θ in equation (B.4) are 0 and $\pi/2$, and equation (B.5) becomes:

$$c = \frac{I}{2\pi\sigma} \tag{B.8}$$

and the potential in the top layer due just to the current injected at point A is:

$$V = \frac{I}{2\pi\sigma_1 r} \tag{B.9}$$

In cylindrical coordinates, where r is the distance from the z-axis, equation (B.9) becomes:

$$V = \frac{I}{2\pi\sigma_1\sqrt{r^2 + z^2}} = \frac{I}{2\pi\sigma_1}\int_0^\infty e^{-kz} J_0(kr)\, dk \tag{B.10}$$

APPENDIX C

Operation of Programs and Sample Outputs

It is assumed that the programs are all compiled using the Microsoft FORTRAN-77 compiler on an IBM PC or compatible computer. The executable programs are then generated by using the Microsoft Linker to link the object code in the following manner:

	PROGRAM	LINKED OBJECT MODULES
1.	ZERO	ZERO, BESDIF
2.	BESCAL	BESCAL, BESDIF
3.	FPPPLT	FPPPLT, QUAD, XI
4.	FOUR	FOUR, QUAD, XI

To run these programs on an IBM PC simply enter the name of the program to be run. ZERO and BESCAL need only be run once to generate the required constants for the other two programs. The following pages show example outputs of the program as run on an IBM PC.

The first program to be run is the program ZERO. The prompts are:

ENTER REQUIRED NUMBER OF DIGITS [DEF = 50]:
(Your response: an integer greater than 0.)
ENTER REQUIRED DIGITS [DEF = 5]: (accuracy)
(Your response: an integer between 1 and 6, inclusive.)
The program proceeds to display the number of zeroes requested, as well as storing them in the file "ZERO.DAT".

The next program is BESCAL. There are no prompts, but the program displays the interval for which it is presently computing the necessary values of $K_1(t)$. These values are stored in the file "TWOBES.DAT".

The third program, FOUR is the program which will be most useful to the researcher. The prompts which appear in this program are:

INITIALIZING QUADRATURE VALUES (reading the files "ZERO.DAT" and "TWOBES.DAT".)

Enter PROBE SPACING <0.159>, cm:
Enter MEASURED VOLTAGE/CURRENT <36.77>, Ω:
Enter THICKNESS of Si <381.00>, μm:
Enter THICKNESS of SiC <6.00>, μm:
Enter RESISTIVITY of SiC <0.22 E + 02>, Ω-cm:
Enter INITIAL GUESS for RESISTIVITY OF SiC <0.1 E + 01>, Ω-cm:
Enter INITIAL DELTA RESISTIVITY <0.1 E + 01>, Ω-cm:
Enter MAXIMUM No. of ITERATIONS <100>:
CHANGES [Y/N] <N>: (if changes are requested the program loops through these prompts again.)

The routines then produces a table similar to the one below:

I	fc	fe	ERR	RHO1
1	1.30009	1.6697	0.22138	0.1000E+00
2	3.69198	1.6697	1.21111	.600E+00
.	.	.	.	.
.	.	.	.	.
.	.	.	.	.
11	1.59509	1.6697	.04470	.1313E+00
12	1.66295	1.6697	.00406	.1391E+00

The calculated SiC RESISTIVITY = 0.13906E+00 Ω-cm.

Following the solution appears the prompt:

ANOTHER MEASUREMENT ? [Y/N] <Y>:
(If the response is "Y" the program returns to the original prompts; if the response is "N" the program ends.)

The fourth program in the package, FPPPLT, is similar in operation to the program FOUR. This routine produces a file which can be used by a package such as "SYMPHONY" to produced plots of the relationship described in this paper. The prompts are:

INITIALIZING QUADRATURE VALUES (reading the files "ZERO.DAT" and "TWOBES.DAT".)

Enter No. of INCREMENTS <20>: (number of points to plot)
Enter PROBE SPACING <1.00>, cm:
Enter THICKNESS of SUBSTRATE <300.00>, μm:
Enter THICKNESS of DEPOSITED LAYER <20.00>, μm:
Enter RESISTIVITY of SUBSTRATE <0.10 E +01>, Ω-cm:
Enter BEGINNING log(RHO1/RHO2) <0.00>:
Enter ENDING log(RHO1/RHO2) <-3.00>:
CHANGES [Y/N] <N>: (if changes are requested the program loops through these prompts again.)

At this point the routine requires a file name under which to store the data. The prompt for this is:

ENTER FOR UNIT 2 THE NAME OF THE OUTPUT FILE
WHICH WILL ACCEPT THE DATA TO BE PLOTTED.
File name missing or blank - please enter name.
UNIT 2? (Your response is to be a legal file name, such as "TEST.DAT".)

REFERENCES

1. Brown, M.A.C.S.; and Jakeman, E.: Theory of the four-point probe technique as applied to the measurement of the conductivity of thin layers on conducting substrates. Brit. J. Appl. Phys., vol. 17, no. 9, Sept. 1966, pp. 1143-1148.

2. Jackson, J.D.: Classical Electrodynamics, 2nd edition, John Wiley and Sons, 1975, p. 30.

3. Panofsky, W.K.H.; and Phillips, M.: Classical Electricity and Magnetism Addison-Wesley, 1962, pp. 28-40.

4. Spiegel, M.R.: Mathematical Handbook of Formulas and Tables, McGraw-Hill, 1968, p. 143.

5. Carnahan, B.; Luther, H.A.; and Wilkes, J.O.: Applied Numerical Methods, John Wiley and Sons, 1969, pp. 101-111.

6. Microsoft FORTRAN Reference Manual, Microsoft Corp., 1984.

7. Symphony Reference Manual, Lotus Development Corp., 1985.

TABLE 1. - COMPARISON OF THEORY WITH EXPERIMENT FOR A BRASS SHIM ON A MERCURY SUBSTRATE

s, cm	λ	W	σ_2, k/(Ω-cm)	ΔV/I, μV/A	Known value	[σ_1 - k/(Ω-cm)] Derived BROWN	Derived FOUR
0.127	4.72	23.2	10.4	63.0	143.0	149.0	150.0
0.063	2.27	19.0	10.4	82.0	141.0	137.0	138.0

Note: k/(Ω-cm); denotes thousands of $(\Omega\text{-cm})^{-1}$, i.e., $1\ \text{k}/(\Omega\text{-cm}) = 10^3\ (\Omega\text{-cm})^{-1}$

Also: For $\sigma = 10\ \text{k}/(\Omega\text{-cm})$
$\rho = 1/\sigma = 10^{-4}, (\Omega\text{-cm})$

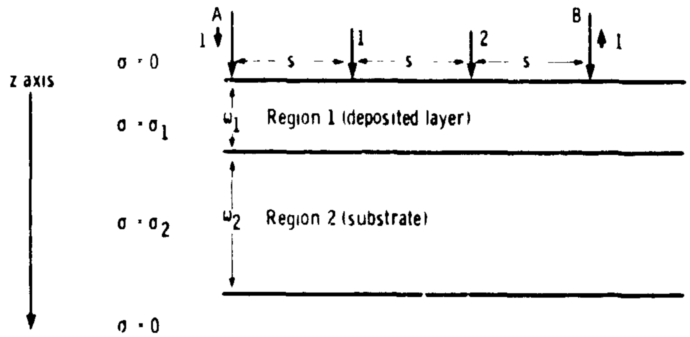
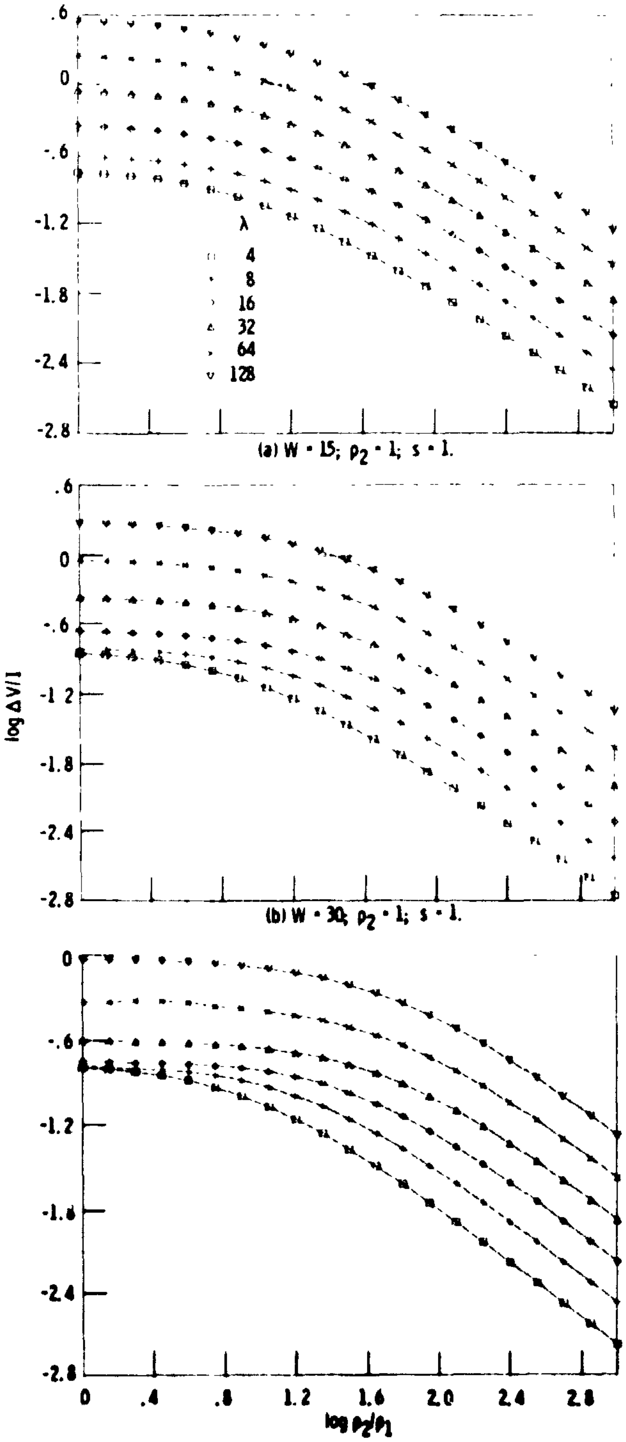


Figure 1. - Theoretical setup for four-point probe measurement of deposited layer on substrate of finite conductivity.



(a) W = 15; ρ_2 = 1; s = 1.

(b) W = 30; ρ_2 = 1; s = 1.

(c) W = 60; ρ_2 = 1; s = 1.

Figure 2. - ΔV/I versus ratio of resitivities.

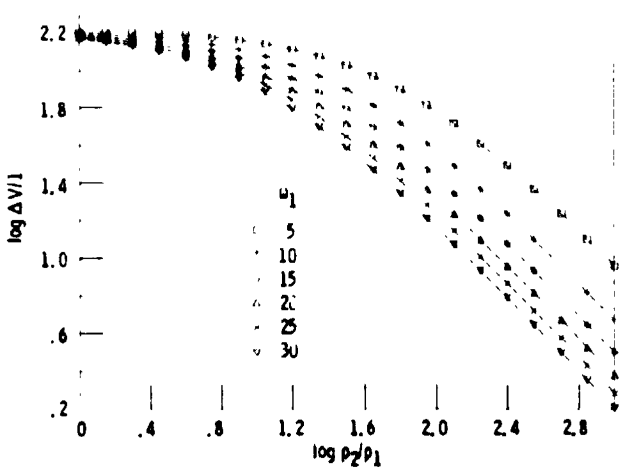


Figure 3. - $\Delta V/I$ versus ratio of resitivities. $\omega_2 = 300$; $s = 0.159$; $\rho_2 = 22$.

1. Report No.
NASA TM-87262

2. Government Accession No.

3. Recipient's Catalog No.

4. Title and Subtitle
A Computer Program to Calculate the Resistivity of a Thin Film Deposited on a Conductive Substrate From Four Point Probe Measurements

5. Report Date
March 1986

6. Performing Organization Code
505-62-01

7. Author(s)
Lawrence G. Oberle and Gustave C. Fralick

8. Performing Organization Report No.
E-2954

9. Performing Organization Name and Address
National Aeronautics and Space Administration
Lewis Research Center
Cleveland, Ohio 44135

10. Work Unit No.

11. Contract or Grant No.

12. Sponsoring Agency Name and Address
National Aeronautics and Space Administration
Washington, D.C. 20546

13. Type of Report and Period Covered
Technical Memorandum

14. Sponsoring Agency Code

15. Supplementary Notes

16. Abstract
A series of FORTRAN-77 programs are described which correct for the effect of a conducting substrate when a linear four-point probe is used to measure the resistivity of a thin film. The resistivity of the film is given in terms of the thicknesses of the film and substrate, the known resistivity of the substrate, and the measured $\Delta V/I$. A full development is given as well as a complete description of the operation of the programs. The programs themselves can be obtained through COSMIC, and are identified as LEW No. 14381.

17. Key Words (Suggested by Author(s))
Four-point probe
Resistivity
Silicon carbide

18. Distribution Statement
Unclassified - unlimited
STAR Category 61

19. Security Classif. (of this report)
Unclassified

20. Security Classif. (of this page)
Unclassified

21. No. of pages

22. Price*

*For sale by the National Technical Information Service, Springfield, Virginia 22161