

Final Technical Report

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"A Study Of The Properties of Beryllium Doped

Silicon With Particular Emphasis On

Diffusion Mechanisms"

Submitted by

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(NASA-CR-129169) A STUDY OF THE PROPERTIES  
OF BERYLLIUM DOPED SILICON WITH PARTICULAR  
EMPHASIS ON DIFFUSION MECHANISMS: PROFILES  
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Final Technical Report

In order to more effectively contribute to the research program of the Instrument Physics Research Section, NASA Langley Research Center, work under this grant was directed toward the problem of measuring diffusion parameters for the beryllium impurity in silicon. The very large ( $\sim 10^{-5} \text{ cm}^2 \text{ sec}^{-1}$ ) diffusion coefficients encountered in this study required the determination of impurity profiles for thick samples ( $\sim 1 \text{ cm}$ ), due to the deep penetration of the impurity occurring during reasonable diffusion times. Since conductivity values are readily converted into concentrations of electrically active impurities, the major problem became that of accurately determining the conductivity profiles of beryllium diffused silicon samples. Details of the problem and its solution are contained in the attached report.

Profiles of Depth Dependent Conductivity  
As Determined by Electrical Surface Probes\*

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Four-point probe measurements on samples having depth dependent conductivities are interpreted in terms of the conductivity profiles. An exact solution of the problem of exponentially depth dependent conductivity serves as a basis for this interpretation. Applications include surface conductivity determination where the form of the conductivity profile is known, and conductivity profile determination from probe measurements taken as the sample surface is progressively lapped away. Application is limited to samples having conductivity monotonically decreasing with depth from the probed surface.

## INTRODUCTION

Electrical surface probes have proven useful in geological exploration<sup>1</sup> as well as in conductivity profile determinations of semiconducting samples.<sup>2,3</sup> Published methods of interpreting surface probe measurements in terms of a depth dependent conductivity are based upon a layered model with conductivity values constant within each layer. These methods use solutions of Laplace's equation within each layer with the implicit assumption that charge accumulations at the boundary are excluded from the layer volume. This neglect of the physical requirement that the charge accumulation occupy a non-zero sample volume gives rise to an error of undetermined magnitude.<sup>3</sup> A second disadvantage of these methods is their complexity which makes consideration of more than a few layers prohibitively difficult.

The four-point probe as illustrated in Fig. 1 is often used in measurements of conductivity. Among its many advantages are ease of application and, for homogeneous or very thin samples, ready interpretation.<sup>4,5</sup> The problem of a slab of finite thickness with an exponentially depth dependent conductivity has been recently solved,<sup>6</sup> and this exact solution serves here as a basis for interpreting four-point probe measurements on samples having other forms of depth dependent conductivity. Applications include surface conductivity determination where the form of the conductivity profile is known, and conductivity profile determination from four-point probe measurements taken as the sample surface is progressively lapped away. In this paper we present a simple method of conductivity profile analysis which appears to be reasonably accurate for samples having a conductivity monotonically

Ref. Fig 1

decreasing with depth from the probed sample surface.

In the following treatment, some of the more important assumptions and stipulations are:

(1) The probe is made up of four collinear contacts with point spacing  $S$ .

(2) The two inner contacts are used to determine the potential difference,  $V$  (volts), due to the current,  $I$  (amperes), through the outer pair of contacts.

(3) Sample conductivity,  $\underline{\sigma}(z)$  [ $\text{ohm-cm}$ ] $^{-1}$ , is a function only of depth below the probed surface.

(4) The probe point spacing is small compared to the probe distance from the nearest lateral boundary.

#### EXPONENTIALLY DEPTH DEPENDENT CONDUCTIVITY

We have shown previously<sup>6</sup> that for conductivities,  $\underline{\sigma}$ , of the form

$$\underline{\sigma}(z) = \underline{\sigma}(0) \exp(-az) , \quad (1)$$

the probe potential difference may be expressed as

$$V = \left[ \frac{I}{2\pi S} \underline{\sigma}(0) \right] F_{aS}(T) , \quad (2)$$

where  $z$  is the depth below the probed surface,  $T$  is the sample thickness, and  $a$  is a constant characterizing a particular exponential depth dependence of the conductivity.  $F_{aS}(T)$  is an appropriate correction

*greek letters  
underlined in  
red*

factor given as

$$F_{aS}(T) = \frac{aS \ln 4}{1 - \exp(-aT)} + \frac{4S}{T} \sum_{n=1}^{\infty} \left( \frac{\ln^2 \pi^2}{\ln^2 \pi^2 + a^2 T^2} \right) \left\{ K_0 \left[ \frac{S}{2T} (\ln^2 \pi^2 + a^2 T^2)^{\frac{1}{2}} \right] - K_0 \left[ \frac{S}{T} (\ln^2 \pi^2 + a^2 T^2)^{\frac{1}{2}} \right] \right\}, \quad (3)$$

where the  $K_0$  are Bessel functions of the zeroth order.

The usefulness of the preceding relationships is greatly enhanced by a recently pseudo-derived approximation to  $F_{aS}(T)$  which is good to within 0.1% error for all  $a \geq 0$ . Our approximation is

$$F_{aS}(T) \approx \frac{aS \ln 4}{1 - \exp(-aT)} + \frac{\exp[-(ST^{-1} \ln 4) - |a| S \ln 2] \operatorname{Tanh} \left\{ (|a| S)^{-1} [\exp(|a| T) - 1] \right\}}{|a| S [\exp(|a| T) - 1]^{-1} \ln 4 + \exp(-ST^{-1} \ln 4)}, \quad (4)$$

which for the case  $a=0$  simplifies to

$$F_{0S}(T) \approx ST^{-1} \ln 4 + \frac{\exp(-ST^{-1} \ln 4) \operatorname{Tanh}(S^{-1} T)}{ST^{-1} \ln 4 + \exp(-ST^{-1} \ln 4)}. \quad (5)$$

The restriction of the approximation to  $a \geq 0$  may be appreciated by verifying that the leading terms of Eqs. (4) and (3) are identical so that the second term of Eq. (4) serves as an approximation to the summation term of Eq. (3). The approximated second term deteriorates as  $|a|$  increases. However, for positive  $a$ , this deterioration is compensated by the increasing dominance of the first term. Unfortunately, for negative  $a$  the approximated term becomes increasingly dominant as  $|a|$  increases.

The function  $F_{aS}(T)$  decreases toward a limiting value as the thickness,  $T$ , increases. This implies that the degree of involvement of the sample material in the conduction process decreases with increasing depth from the probed surface. For sample thicknesses small compared to the probe spacing, the effect of sample material upon the probe potential is almost independent of depth below the probed surface and the leading term of  $F_{aS}(T)$  dominates. In this case Eq. (2) reduces to the expression<sup>5</sup>

$$V = (\ln 2/\pi) (I/\sigma_s) , \quad (6)$$

appropriate for a thin infinite sheet having sheet conductivity,  $\sigma_s$ . For our purposes, we find it convenient to extend the range of Eq. (6) to any thickness by introducing a multiplicative factor,  $W_{aS}(z)$ , into the usual definition of sheet conductivity so that

$$\sigma_s = \int_0^T W_{aS}(z) \sigma(z) dz. \quad (7)$$

Combining Eqs. (6) and (7) to obtain

$$\int_0^T W_{aS}(z) \sigma(z) dz = (\ln 2/\pi) (I/V) , \quad (8)$$

we observe that a knowledge of  $(I/V)$  as a function of either  $S$  or  $T$  uniquely determines  $\sigma(z)$ .

Since Eqs. (2) and (6) both describe the same situation, we must have

$$\int_0^T W_{aS}(z) \underline{\sigma}(z) dz = S \ln 4 \underline{\sigma}(0) F_{aS}^{-1}(T) . \quad (9)$$

We assume that the degree of involvement of the material at a given depth in the conduction process is solely dependent upon the conductivity and thickness of the overlying material. The mathematical implication of this assumption is that the weighting factor  $W_{aS}(z)$ , in the left hand term of Eq. (9) is independent of the limit of integration, T. Thus we may differentiate the terms of Eq. (9) with respect to T to obtain

$$W_{aS}(z) = S \ln 4 \underline{\sigma}(0) \underline{\sigma}^{-1}(z) \left[ \partial F_{aS}^{-1}(z) / \partial z \right] . \quad (10)$$

Some representative weighting functions appropriate to samples having exponentially depth dependent conductivities are shown in Fig. 2.

While the assumption of the preceding paragraph is not strictly valid, it appears to be a good approximation to reality in the case of semiconductor slabs having the conductivity decreasing as the depth below the probed surface increases. It may be helpful to examine an equivalent assumption that the conduction process at depths greater than z has no effect upon the electric field at depth z. This clearly suggest that our assumption is far from valid when the underlying material is of relatively high conductivity.

For interpreting four-point probe measurements made as the top sample surface is progressively lapped away, we are pleased to note that  $W_{OS}(z)$  serves as a useful approximation to all  $W_{aS}(z)$ ,  $a \geq 0$ . Replacing  $W_{aS}(z)$  by  $W_{OS}(z)$  in application of Eq. (8) to constructs devised using a wide range of exponential dependencies, the maximum error encountered in surface conductivity,  $\underline{\sigma}(0)$ , was less than 6%.

This magnitude of cumulative error has little effect upon the form of the profile. The maximum error occurs for large sample thickness and at a conductivity profile characterized by the exponential factor  $a=S^{-1}$ . This error in sample surface conductivity goes rapidly to zero as  $a$  approaches zero and has decreased to 0.6% at  $a=5S^{-1}$ . This is consistent with the observation that the true weighting function,  $W_{aS}(z)$ , will be significantly higher than  $W_{OS}(z)$  only when the material overlying the region about  $z$  has a relatively high conductivity; or equivalently only when the material about  $z$  has a relatively low conductivity so that the effect of the material at  $z$  upon the probe potential is relatively unimportant.

#### APPLICATION

The modified concept of sheet conductivity, as seen in Eq. (7), can be readily extended to other forms of depth dependence of conductivity, subject only to the availability of an appropriate weighting factor. For samples not having exponentially depth dependent conductivities, the weighting function,  $W_S(z)$ , must of necessity be an approximation. The use of the weighting function  $W_{aS}(z)$  for samples having conductivity profiles characterized by  $a$  introduces no computational error and one might expect that for samples having conductivity profiles similar in form to an exponential depth dependence, the use of an appropriate  $W_{aS}(z)$  would produce highly accurate results.

The primary motivation for this study was the need of a convenient and reliable method of determining concentration profiles of impurities diffused into semiconductors. Conductivity values are readily converted into concentrations of electrically active impurities using mobility

data such as that summarized by E. M. Conwell.<sup>7</sup> In silicon, typical diffusion depths of substitutional impurities are a few microns and the easily applied four-point probe method offers high resolution and ready interpretation.<sup>5,8</sup> Penetration depths of the fast diffusing interstitial impurities are measured in millimeters, however, and require use of a more complex interpretation of four-point probe data.

To accomplish a conductivity profile analysis we may consider the sample to be an N-layered structure as illustrated in Fig. 3. Layers are characterized by an average conductivity  $\bar{\sigma}_i$ , a thickness  $(\Delta T)_i$ , and an average weighting factor  $\bar{W}_{Si}$ . The generalized form of Eq. (8), in a form suitable for numerical integration, is

$$\sum_{i=1}^N \bar{W}_{Si} \bar{\sigma}_i (\Delta T)_i = (\ln 2 / \pi) (I/V)_S. \quad (11)$$

By applying Eq. (11) to surface measurements taken with N different probe-point spacings, we obtain N equations with N unknown  $\bar{\sigma}_i$ .

Calculation is simplified in cases where four-point probe measurements are made on the top sample surface at each stage as the layers are progressively lapped away. In this case we use a constant probe spacing and obtain the average conductivity of the  $j^{\text{th}}$  layer as

$$\bar{\sigma}_j = \left[ (\ln 2 / \pi) (I/V)_j - \sum_{i=1}^{j-1} \bar{W}_{Si} \bar{\sigma}_i (\Delta T)_i \right] \left[ \bar{W}_{Sj} (\Delta T)_j \right]^{-1}. \quad (12)$$

It should be clear that the calculations must begin with the sample remnant and work back toward the first layer to be removed.

It is sometimes desirable to find the value of the surface conductivity of a sample for which the form of the depth dependent conductivity profile

is already known. Rewriting  $\underline{\sigma}(z)$  as  $\underline{\sigma}(0)f(z)$  in Eq. (8) and solving for the surface conductivity,  $\underline{\sigma}(0)$ , we obtain

$$\underline{\sigma}(0) = (I/V)_S (\ln 2/\pi) \int_0^T W_S(z) f(z) dz . \quad (13)$$

For application of Eqs. (12) and (13) we take  $W_{OS}(z)$ , the weighting function appropriate to a homogeneous sample, as a fair approximation to the true  $W_S(z)$  for all samples having conductivities decreasing monotonically with increasing depth from the top surface. As in our previous discussion of the  $W_{aS}(z)$ , this assumption is consistent with our expectation that the true  $W_S(z)$  will be significantly higher than  $W_{OS}(z)$  only when the overlying material has a rather high conductivity relative to the material at depth  $z$ , so that the effect of the material at depth  $z$  upon the probe potential is relatively unimportant.

In addition to the theoretical constructs involving constant and exponentially depth dependent conductivities, conductivity profiles due to gaussian and complimentary error function distributions of impurities in silicon have been employed to verify the usefulness of Eq. (12) in making profile analyses. Eq. (12) is being used extensively in studies of the beryllium impurity in silicon and yields impurity concentration profiles consistent with those expected from imposed experimental conditions<sup>9</sup> and with those obtained by mass spectroscopy analysis.

In Fig. 4 we see the results of a 27 layer determination of the concentration profile of electrically active beryllium as a diffused impurity in silicon. The beryllium was introduced into the silicon at high temperature from one side only. The experimentally determined concentrations are shown fitted to the expected complimentary error function profile.

## List of References and Footnotes

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## Captions for Figures

Fig. 1. Four-point probe on flat semiconductor.

Fig. 2. Some representative weighting functions,  $W_{aS}(z)$ , appropriate for samples having depth dependent conductivities of the form  $\sigma(z) = \sigma(0) \exp(-az)$ . Units are chosen such that  $S = 1$ .

Fig. 3. Multi-layered sample geometry assumed for conductivity profile determinations.

Fig. 4. A 27 layer determination of the concentration profile,  $N(z)$ , of electrically active beryllium as a diffused impurity in silicon.







