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# THE RELATIONSHIPS BETWEEN SURFACE CHARGE AND DIFFUSION POTENTIAL BENEATH SEMICONDUCTOR SURFACES

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# THE RELATIONSHIPS BETWEEN SURFACE CHARGE AND DIFFUSION POTENTIAL BENEATH SEMICONDUCTOR SURFACES\*

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### Introduction

In this paper the potential change at the boundary between a semiconductor or an insulator and a gas or vacuum phase is formulated as a function of the concentration of ionized donor or acceptor centers on the surface of a one-dimensional, semi-infinite plane. for all combinations of the types of semiconductors and the ions on the surface. This covers the majority of cases wherein the diameter of the solid particle is equal to or greater than  $10^{-4}$  cm. The surface then can be considered as a plane with a thickness extending to infinity relative to the space charge region underneath the surface of the semiconductor. Hauffe and Engell have referred to this potential as a "diffusion potential" when it is defined in the interior of a material but the term "surface potential" has been used by Buck and others working on semiconductor surfaces to define the diffusion potential at a surface. These relations will be used in a subsequent publication to derive additional mathematical expressions for adsorption isotherms of gases on semiconductor surfaces, when charge trans-

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fer occurs during the adsorption.

A second objective of this paper is to clarify the previous literature on the subject of the diffusion potential inside a semiconductor. Many authors have formulated relationships between the surface ion concentration and diffusion potential for some special cases. Aigrain and Dugas, Hauffe and Engell, Weisz, and Garrett and Brattain<sup>5</sup> all have derived relationships and discussed depletion or inversion layers on semiconductor surfaces. Kingston and Neustadter and Young have used numerical integration to calculate the space charge and diffusion potential relationships. Bohnenkamp and Engell<sup>8</sup> later derived an analytic expression for the space charge variation with distance for a special case. These last authors have tacitly assumed that the semiconductor has a semi-infinite extension, and applied Gauss's Law to calculate the space charge. In this paper all these derivations are placed in context as being representative of certain special cases, and are mentioned in the appropriate sections. The assumption has been made that the diffusion potential tends to zero in the bulk semiconductor, and the variation of the diffusion potential with distance from the surface is investigated.

In order to derive the appropriate relationships, Poisson's equation for the one-dimensional case must be solved.

$$\frac{d^2 E(x)}{dx^2} = \frac{4\pi q^2 P(x)}{\epsilon}$$
 (1)

where

q  $\rho(x)$  = bulk charge density, positive charges/cm<sup>3</sup>.  $[\rho(x)]$  is at least a sectionally continuous function of x. Note that this will include the case wherein there is a surface charge.  $[\rho(x)]$  = electron energy, eV.

 $-\frac{1}{q}E(x)$  = electrostatic potential at x, volts.

 $\epsilon$  = dielectric constant.

q = unit positive charge,  $1.6 \times 10^{-19}$  coulombs.

x = distance into the bulk region of the semiconductor, from the surface, cm.

The total charge density inside the semiconductor (algebraic sum of all fixed charge and all mobile charge) arises from ionized donors and acceptors, and from holes and electrons. The net concentration of positively charged species then is

$$\rho(x) = (N_d^{\dagger} - N_{\bar{d}}) + p(x) - n(x)$$
 (2)

 $N_a^-$  = concentration of acceptor centers in the bulk, acceptors/cm<sup>3</sup>.

 $N_d^{\dagger}$  = concentration of donor centers in the bulk, donors/cm<sup>3</sup>.

 $p(x) = \text{hole concentration at } x, \text{ holes/cm}^3.$ 

n(x) = electron concentration at x, electrons/cm<sup>3</sup>.

Equations (1) and (2) must be obeyed within the semiconductor.

On the surface the net surface charge then is

$$q \sigma_{\mathbf{D}} = q \left( \sum \mathbf{j} D^{\mathbf{j}} - \sum \delta A^{\delta -} \right)$$
 (3)

where

 $q \sigma_{\Box} = \text{net positive surface charge, coulombs/cm}^2$ .

 $D^{\gamma}$  = ionized donors with valence state  $\gamma$ , donors/cm<sup>2</sup>.

 $A^{\delta-} = \text{ionized acceptors of valence state } \delta, \text{ acceptors/cm}^2.$  (The summation is carried out for all possible  $\gamma$  and  $\delta$ ).

By the principle of conservation of charge (electro-neutrality) the following equation must be obeyed:

$$\sigma_{\square} + \int_{0}^{\infty} \rho(x) dx = 0$$
 (4)

$$-\int_{0}^{\infty} \rho(x) dx = \sigma_{D} = (\sum \gamma) D^{\gamma} + -\sum \delta A^{\delta-})$$
 (5)

Equations (1), (2), and (4) are required to express the surface potential as a function of the concentration of surface centers. In Equation (5) it is assumed that the effects of charges on the surface extend to infinity into the interior of the semiconductor.

In order to investigate all possible interrelationships between the charge on the surface and the electrical nature of the semiconductor, it is necessary to consider three groups of cases which increase in mathematical complexity. The first group of two cases can be defined for surface donors or acceptors on an intrinsic semiconductor. The second group of two cases can be defined for surface donors on an n-type semiconductor, and for surface acceptors on a p-type semiconductor. In these cases accumulation layers are formed underneath the semiconductor surfaces. The third group of six cases can be defined for surface donors on a p-type semiconductor or for surface acceptors on an n-type semiconductor. Three pairs of cases can be defined in this group depending on whether the surface layers are depletion layers intrinsic, or inversion layers.

### A. Intrinsic Semiconductors (Including Insulators).

Either donor centers or acceptor centers on the surface can be considered under this category. In these cases the donor and acceptor concentrations inside the crystal are small relative to the intrinsic carrier concentrations.

$$(N_d^{\dagger} - N_a^{-}) \ll n_i = p_i$$

Therefore from Equation (2)

$$Q(x) = [p(x) - n(x)]$$
(6)

### Case 1. Surface Donors on an Intrinsic Semiconductor.

For the case of surface donors on an intrinsic semiconductor the surface charge density from Equation (5) can be simplified as

$$\sigma_{\mathbf{D}}^{+} = \sum_{i} (\gamma) D^{\gamma + i}$$
 (7)

If it is assumed that the semiconductor is in a non-degenerate condition and the Boltzmann statistics are applicable, then the hole and electron concentrations in the space-charge region can be written as:

$$(x) = p_i \exp \left[-(E_f - E_g(x)/2)/kT\right] = p_i \exp \left[-Y(x)/kT\right] = p_i \exp(-u) (8a)$$

$$n(x) = n_i \exp \left[ (E_f - E_g(x)/2)/kT \right] = n_i \exp \left[ Y(x)/kT \right] = n_i \exp u$$
 (8b)

where

$$Y(x) = \begin{bmatrix} E_{C_B} - E_{C}(x) \end{bmatrix} = \begin{bmatrix} E_{V_B} - E_{V}(x) \end{bmatrix} = \begin{bmatrix} E_{i_B} - E_{i}(x) \end{bmatrix}$$

 $u = Y(x)/kT = normalized diffusion potential, (kT) units. The sign of Y(x) then is taken as positive when the surface becomes more n-type as shown in Figure 1. Furthermore, since the bulk material is an intrinsic semiconductor, then <math>n_i = p_i$ , where  $n_i$  and  $p_i$  are the equilibrium intrinsic electron and hole concentrations in the bulk of the semiconductor, respectively. Furthermore, since

$$\frac{d^2 u}{dx} = \frac{1}{kT} \quad \frac{d^2 Y(x)}{dx} = -\frac{1}{kT} \quad \frac{d^2 E(x)}{dx}$$
(9)

then Equations (8) and (9) can be substituted into Equation (1) to give an alternate expression for Poisson's Equation.

$$\frac{d^{2}u}{dx^{2}} = -2 L_{m} \rho(x) = 4 L_{m} n_{i} \sinh u$$
 (10)

where Equation (10) has been simplified by defining  $\boldsymbol{L}_{\boldsymbol{m}}$  as

$$L_{\rm m} = \frac{2\pi q^2}{\epsilon kT} \quad \text{(in cm)} \tag{11}$$

Now the variable on the left side of Equation (10) can be changed from  ${\bf x}$  to  ${\bf u}$ , since

$$\frac{d^{2}u}{dx^{2}} = \frac{d}{dx} \left(\frac{du}{dx}\right) = \frac{du}{dx} \frac{d}{du} \left(\frac{du}{dx}\right)$$
$$= \frac{1}{2} \frac{d}{du} \left[\left(\frac{du}{dx}\right)^{2}\right]$$

Therefore

$$\frac{1}{2} \frac{d}{du} \left[ \left( \frac{du}{dx} \right)^2 \right] = 4L_{mi} \sinh u = -2L_{mi} (u)$$
 (12)

In order to integrate this equation, appropriate boundary conditions must be established.

In the bulk semiconductor, far away from the surface where  $n = n_i = p_i = p$ , the following boundary conditions can be established:

$$\lim Y(x) = 0, \text{ or } u = 0 \text{ at } x = \infty$$
 (13)

 $x \rightarrow \infty$ 

$$\lim_{x \to \infty} \frac{d Y(x)}{d x} = 0, \text{ or } \frac{du}{d x} = 0 \text{ at } x = \infty$$
(14)

The boundary condition at x = 0 can be defined as:

$$u = u_S, \text{ at } x = 0 \tag{15}$$

By applying the boundary condition from Equations (13) and (14) at  $x = \infty$ , and integrating Equation (12), it follows that

$$\left(\frac{\mathrm{du}}{\mathrm{dx}}\right)^2 = 8L_{\mathrm{m}} n_{\mathrm{i}} \left[\cosh u - 1\right] \tag{16}$$

Furthermore, Equation (16) can be simplified by using the identity

$$\cosh u - 1 = 2 \sinh^2 (u/2)$$
 (17)

Combining Equations (16) and (17) and taking the square root gives

$$\frac{du}{dx} = \pm 4 \left( L_{mn} \right)^{1/2} \sinh \left( u/2 \right) \tag{18}$$

Since a surface donor lowers the edges of the bands, then

 $\frac{dE}{dx}$  = positive. However, Y(x) decreases (from its definition) and the negative sign must be chosen in Equation (18). Therefore,

$$\frac{du}{dx} = -4 \left( L_{mn_i} \right)^{1/2} \sinh \left( u/2 \right) \tag{19}$$

# a. The Surface Potential, $u_s$ .

In order to express the surface potential,  $u_s$ , in terms of the surface charge,  $\sigma_D$ , the conservation of charge relation (Equation 4) can be substituted into Poisson's Equation, Equation (10).

By using the boundary conditions defined in Equations (5) and (14), this can be integrated.

$$\frac{du}{dx} \Big|_{x=0}^{x=\infty} = -2L_{m} \int_{0}^{\infty} (x) dx$$

The result is

$$-\left(\frac{\mathrm{du}}{\mathrm{dx}}\right)_{\mathrm{O}} = 2L_{\mathrm{m}} \sigma_{\mathbf{D}}^{+} \tag{20}$$

From Equation (19), when  $u = u_s$ , at x = 0, the derivative of the diffusion potential at the surface can be found and substituted into Equation (20).

Therefore

$$\sinh (u_s/2) = \frac{2L_m \sigma_D}{4L_m^{1/2} n_i^{1/2}} = \frac{\sigma_D L_m^{1/2}}{2n_i^{1/2}}$$

or

$$\sinh (u_s/2) = \frac{1}{2} \left(\frac{L_m}{n_i}\right)^{1/2} \sigma_0^+$$
 (21)

This equation has also been derived by Bohnenkamp and Engell.  $^{8}$ 

Under the condition that  $E_s/kT = u_s > 2$ 

$$\sinh \left(\frac{u_s}{2}\right) \stackrel{\sim}{\sim} \frac{1}{2} \exp \left(u_s/2\right)$$

Therefore

$$\exp (u_s/2) = (\frac{L_m}{n_i})^{1/2} \sigma_n^+$$

Taking the logarithm gives

$$u_{s} = \frac{Y_{s}}{kT} = \ln \left\{ \frac{L_{m}}{n_{i}} \sigma_{n}^{+2} \right\}$$
 (22)

This result can be written alternately as

$$u_{s} = \frac{Y_{s}}{kT} = \frac{Eg}{kT} + \ln \frac{L_{m} \sigma_{n}^{+2}}{\sqrt{N_{c} N_{v}}}$$
 (23)

The magnitude of the surface potential on an intrinsic semiconductor then depends directly on the energy gap of the substrate and logarithmically on the surface charge density.

## b. The Diffusion Potential, u(x).

The variation of the diffusion potential as a function of distance from the surface inside the semiconductor can be determined by integrating Equation (19). The identity

$$d \left\{ \ln \left[ \tanh \left( \xi \right) \right] = \frac{d \xi}{\sinh \xi \cosh \xi} = \frac{2d \xi}{\sinh 2\xi}$$

can be substituted into Equation (19) and the variables separated for integration.

$$\frac{du}{\sinh(u/2)} \stackrel{\mathbf{2}}{=} -4 \left(L_{m} n_{i}\right)^{1/2} dx \tag{24}$$

By using the boundary condition defined by Equation (15) the result is

$$\ln \left[ \frac{\tanh (u/4)}{\tanh (u_s/4)} \right] = -2 (L_m n_i)^{1/2} x$$

Written in alternate form:

$$tanh (u/4) = tanh (u_s/4) exp (-2x \sqrt{L_m n_i})$$
 (25)

where  $u_s$  must be evaluated by Equations (21) or (22).

if 
$$u_s/4 \gg 1$$
,  $\tanh (u_s/4) \approx 1$ .  
 $\tanh (u/4) \approx \exp (-2x\sqrt{L_m n_i})$  (26)

When  $(u/4) \ll 1$ , (i.e., deep in the bulk)

$$tanh(u/4) = u/4 - \frac{(u/4)^2}{3} + \dots$$

Therefore

$$u(x) = 4 \exp(-2x \sqrt{L_{m_i}^n})$$
 (27)

This equation indicates that the diffusion potential, u, decreases exponentially as x increases into the interior region of the semiconductor in a manner which is independent of the surface potential. (Mott and Gurney  $^9$  have derived this equation to explain the potential barrier which exists at the interface between two solids.)

Since  $n_i$  is an exponential function of temperature, Equation (27) shows that the diffusion potential decreases as an exponential function of an exponential function, as the temperature increases.

### Case 2. Surface Acceptors on an Intrinsic Semiconductor.

Now consider the intrinsic semiconductor with acceptors on the surface. The surface charge density is given as

$$\mathcal{T}_{\square} = \mathcal{T}_{\square}^{-} = -\sum (\delta A^{\delta-})$$
(7a)

Since acceptors on the surface tend to make the space charge region become p-type, then the surface potential must be inherently negative in this situation. Therefore, in order to deal with positive values of the surface potential and the diffusion potential in the equations, primed values are defined such that

$$u' = -u$$
 and  $u'_s = -u_s$ 

The expression for the surface potential is

$$\sinh (u_s/2) = \frac{1}{2} (L_m/p_i)^{1/2} \sigma_{\bar{p}}$$
 (21a)

When  $u_s'$  is greater than 2, then

$$u'_{S} = \ln \left\{ \frac{L_{m}}{p_{i}} \left( \overline{O_{D}} \right)^{2} \right\}$$
 (22a)

The variation of the diffusion potential with distance below the surface is

$$\tan (u'/4) = \tanh (u'/4) \exp (-2x \sqrt{L_{m}p_{i}})$$
 (25a)

Deep in the interior of the semiconductor

$$u(x) \stackrel{!}{\sim} 4 \exp(-2x \sqrt{L_{m}p_{i}})$$
 (27a)

The results for surface acceptors on an intrinsic substrate then are only trivially different from the results obtained for surface donors on an intrinsic substrate.

# B. Accumulation Space Charge Regions on Extrinsic Semiconductors.

Under this title either an n-type semiconductor with donor centers on the surface, or a p-type semiconductor with acceptor centers on the surface, can be considered. The first situation will be presented in detail and the results which are obtained by repeating the derivation for surface acceptors on a p-type semiconductor will be summarized.

#### Case 3. Surface Donors on an n-type Semiconductor.

In the case of an n-type semiconductor it can be assumed that the acceptor concentration in the bulk region is negligible in comparison with the donor: concentration. An energy band diagram for this situation is shown in Figure 2. Equation (2) becomes

$$\rho(x) = (N_d^+) + p(x) - n(x)$$
 (28)

The surface charge density is expressed by Equation (5), and the hole and electron concentrations can be related to the diffusion potential

$$p(x) = p_B \exp(-u), n(x) = n_B \exp u$$
 (29)

where

 $p_B$ ,  $n_B$  = the bulk hole and electron concentrations, respectively, carriers/cm.<sup>3</sup>

Let

$$\exp u_B = \sqrt{n_B/p_B}; \exp (-u_B) = \sqrt{p_B/n_B}$$
 (30)

Note also that  $(p_B^n)^{1/2} = n_i = p_i$  = intrinsic concentration of electrons or holes. The factor  $u_B$  then is the displacement of the Fermi level from the mid-band position. Therefore the charge density in the interior can be expressed by substituting these definitions into Equation (2), and the result is

$$(x) = (N_{d}^{+}) + n_{i} \left\{ \exp(-u_{B}) \exp(-u) - \exp(u_{B}) \exp u \right\}$$

$$= (N_{d}^{+}) - 2 n_{i} \sinh(u_{B} + u)$$
(31)

In the bulk region of the semiconductor where  $\rho(x) = 0$  then it follows that

$$sinh u_B = (N_d^{\dagger}) / 2 n_i$$
 (32)

When Equation (31) is substituted into Poisson's Equation, Equation (12), the resulting equation can be integrated using the boundary conditions defined in Equations (13) and (14) at  $x = \infty$ . The result is

$$\left(\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}\mathbf{x}}\right)^2 = 4 L_{\mathrm{m}} \left\{ 2 n_{\mathrm{i}} \cosh \left(\mathbf{u}_{\mathrm{B}} + \mathbf{u}\right) - 2 n_{\mathrm{i}} \cosh \mathbf{u}_{\mathrm{B}} - \left(N_{\mathrm{d}}^{\mathrm{i}}\right) \mathbf{u} \right\}$$
(33)

The hyperbolic functions in this equation must be resolved through identities. In order to do this, let

$$\mathbf{f} = \mathbf{u}_{B} + \mathbf{u}/2$$
 and  $\eta = \mathbf{u}/2$ 

Then recall

$$\cosh (\xi + \gamma) - \cosh (\xi - \gamma) = 2 \sinh \xi \sinh \gamma$$
Therefore

$$\cosh (u_B + u) - \cosh u_B = 2 \sinh (u/2) \sinh (u_B + u/2)$$
 (34)

Also

 $\sinh (u_B + u/2) = \cosh u_B \sinh (u/2) + \cosh (u/2) \sinh u_B$ This can be written alternately as

$$\sinh (u_B + u/2) = \frac{2 \exp u_B + \exp (-u_B) - \exp u_B}{2} \sinh (u/2)$$

$$+\frac{2 \exp{(-u/2)} - \exp{(-u/2)} + \exp{(u/2)}}{2} \sinh u_B$$

Therefore

$$\sinh (u_{R} + u/2) = \exp u_{R} \sinh (u/2) + \exp (-u/2) \sinh u_{R}$$
 (35)

Substitution of Equation (35) into (34) gives

$$\cosh (u_B + u) - \cosh u_B = 2 \sinh (u/2) \left\{ \exp u_B \sinh (u/2) + \exp (-u/2) \sinh u_B \right\}$$

When this result is substituted into Equation (33) it follows directly that

$$\left(\frac{du}{dx}\right)^{2} = 4 L_{m} \left\{ 4 n_{i} \exp u_{B} \left[ \sinh(u/2) \right]^{2} + 2 n_{i} \left[ 1 - \exp(-u_{B}) \right] \sinh u_{B} - \left(N_{d}^{+}\right) u \right\}$$
(36)

This equation now can be used as a basis for deriving the surface potential and the diffusion potential.

# a. The Surface Potential, $u_s$ .

In order to evaluate the surface potential,  $u_s$ , assuming that it is somewhat larger than kT, then the exponential term in the  $\sinh^2(u/2)$  dominates Equation (36). By evaluating the slope at x=0 and taking the square root with the negative sign, the result is

$$\left(\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}\mathbf{x}}\right) \approx \sqrt{4 \, \mathbf{L}_{\mathrm{m}}} \left\{4 \, \mathbf{n}_{\mathrm{i}} \, \exp \, \mathbf{u}_{\mathrm{B}} \left[\sinh \left(\mathbf{u}_{\mathrm{s}}/2\right)\right]^{2}\right\}^{1/2} = -4 \sqrt{\mathbf{L}_{\mathrm{m}} \mathbf{n}_{\mathrm{B}}} \sinh(\mathbf{u}_{\mathrm{s}}/2) \quad (37)$$

By combining Equation (20) with Equation (37) the result is

$$\sinh (u_s/2) = \frac{1}{2} \left(\frac{L_m}{n_B}\right)^{1/2}$$
 (38)

If  $(u_s/2)$  is much greater than unity so that the hyperbolic sine can be approximated by an exponential, then

$$u_{s} = \ln \left\{ \frac{L_{m}}{n_{B}} \left( \sigma_{\mathbf{D}}^{+} \right)^{2} \right\} = -u_{B} + \ln \left\{ \frac{L_{m}}{n_{i}} \left( \sigma_{\mathbf{D}}^{+} \right)^{2} \right\}$$
(39)

These expressions for surface potential are very similar to those which were derived for the intrinsic semiconductor, and differ only by the change in reference carrier concentration from  $\mathbf{n}_i$  to  $\mathbf{n}_B$ . The surface potential then is reduced by an amount equal to the bulk diffusion potential,  $\mathbf{u}_B$ .

# b. The Diffusion Potential, u(x).

To investigate the diffusion potential, u(x), within the semiconductor consider two limiting subcases. In the first subcase to be considered, Equation (36) is represented by a first order approximation for all values of u. In the second subcase, a second order approximation is made for small values of u only.

# Subcase 3a. First order approximation, for all u(x).

If u(x) is large then the exponential factor in the  $sinh^2$  term is dominant in Equation (36). After taking the square root with the negative sign it becomes

$$\frac{du}{dx} = -4 \left( L_{m} n_{B} \right)^{1/2} \sinh \left( u/2 \right) \approx -2 \left( L_{m} n_{B} \right)^{1/2} \exp \left( u/2 \right) \tag{40}$$

The variables can be separated in this equation, and integration of the exponential form using the boundary condition from Equation (15) gives

$$\exp(-u/2) - \exp(-u_s/2) = x(L_m n_B)^{1/2}$$

Therefore

$$u(x) \cong 2 \ln \left[ \frac{1}{\exp(-u_s/2) + x(L_m n_B)^{1/2}} \right]$$
 (41)

If the sinh form is retained, then a more tractable solution is obtained, which is

$$tanh (u/4) \approx tanh (u_s/4) \exp -2 \times (L_m n_B)^{1/2}$$
 (42)

If  $u_{s} \rightarrow 4$ , so that  $tanh (u_{s}/4) \approx 1$ , then

$$\tanh (u/4) \approx \exp -2 \times (L_{m} n_{B})^{1/2}$$
 (43)

and the variation of the diffusion potential with distance is obtained.

Now if u is small, so that  $[1 - \exp(-u)] \approx u$ , then the resulting approximation from Equations (36) and (32) is also equal to Equation (40). Therefore Equation (40) is a fair approximation throughout the space charge region since sinh (u/2) is a monotonically increasing function.

Equation (43) now can be used to define u (x) over all regions of x. When u becomes small such that  $tanh (u/4) \stackrel{\checkmark}{\smile} u/4$ , then

$$u(x) \approx 4 \exp - 2 \times (L_m n_B) 1/2$$
 (44)

Equations (41) through (44) then represent the variation of the diffusion potential with distance using the first order approximations.

### Subcase 3b. Second order approximation for small u.

If u is small, then

$$\cosh u \approx 1 + \frac{u^2}{2!}$$

 $sinh u = u (u^3 and higher are neglected)$ 

and these approximations can be inserted into Equation (33). Since

 $\cosh (u_B + u) = \cosh u_B \cosh u + \sinh u_B \sinh u$  the above second order approximations give

$$\cosh (u_B + u) = \cosh u_B + \frac{u^2}{2} \cosh u_B + (\sinh u_B) u \qquad (45)$$

Combine Equations (32), (45) and (33). After taking the square root and using the negative sign since u is the dimensionless electron potential energy defined in Figure 2 which is decreasing to zero as x approaches to infinity, the resulting equation is

$$\left(\frac{du}{dx}\right) = -2 \left(L_{m} n_{i} \cosh u_{B}\right)^{1/2} u \tag{46}$$

Therefore integrating Equation (46)

$$u(x) = (constant) \exp \left[-2 \left(L_{m}^{n} n_{i} \cosh u_{B}\right)^{1/2} x\right]$$
 (47)

Since

cosh 
$$u_B = \frac{1}{2} (\exp u_B + \exp - u_B)$$
  
=  $\frac{1}{2n_i} (p_B + n_B)$ 

This identity can be substituted into Equation (47).

$$u(x) = (constant) exp - \left[2L_m(p_B + n_B)\right]^{1/2} x$$
 (48)

Note that Equation (48) has the same form as Equation (27) when  $n_B = p_B = n_i$  except that the constant of integration has not yet been evaluated in Equation (48). By comparing Equation (48) with Equation (44) it appears that u(x) decreases faster in Equation (44) for heavily or moderately doped semiconductors wherein the minority carrier concentration can be neglected. At the same time, these two equations do not become identical short of infinity, and the integration constant in Equation (47) cannot be evaluated readily. The second order approximation, however, would probably be preferred to give the shape of the diffusion potential variation over the region in which it is applicable.

#### Case 4. Surface Acceptors on a p-Type Semiconductor

In this case the energy band diagram is shown in Figure 3. The surface charge density is given by Equation (7a). Also for a p-type semiconductor, let

$$u_{B'} = \ln \left( \frac{p_{B}}{n_{B}} \right)^{1/2} = -u_{B}$$
 (30a)

Therefore the bulk charge density variation can be expressed as

$$\rho(u') = -(N_a) + 2 n_i \sinh(u_B' + u') = -(N_a) - n_i \sinh(u_B + u)$$
 (31)

An analysis similar to Case 3 shows that the surface potential is related to the surface charge density through the relationships

$$\sinh (u_{s'}/2) = \frac{1}{2} \left(\frac{L_{m}}{p_{B}}\right)^{1/2} (\sigma_{D}^{-})$$
 (38a)

For large  $u_s'$ :

$$u_s' \simeq \ln \left\{ \frac{L_m}{p_B} \left( \sigma_D^{-} \right)^2 \right\} = -u_B' + \ln \left\{ \frac{L_m}{n_i} \left( \sigma_D^{-} \right)^2 \right\}$$
 (39a)

The diffusion potential can be found from the relationships as follows:

For large values of u(x)

$$u'(x) \approx 2 \ln \left\{ \frac{1}{\exp (u_s'/2) + x (L_m p_B)^{1/2}} \right\}$$
 (41a)

Also for large values of u(x)

$$tanh (u'/4) \approx tanh (u'/4) exp - 2x (L_m p_B)^{1/2}$$
 (42a)

For  $u_s' >> 4$ , so that  $tanh (u_s'/4) \approx 1$ , then

$$\tanh (u'/4) \approx \exp \left\{-2 \times (L_{m}p_{B})^{1/2}\right\}$$
 (43a)

For large x and small u (x), then the first order approximation gives

$$u' \simeq 4 \exp -2 \times (L_m p_R)^{1/2}$$
 (44a)

and the second order approximation gives

u' 
$$\simeq$$
 (constant) exp  $-x \left[2 L_{m} (p_{B} + n_{B})\right]^{1/2}$  (47a)

#### C. Depletion-Inversion Space Charge Regions on Extrinsic Semiconductors

Under this title the combinations of a p-type semiconductor with donor centers on the surface, and an n-type semiconductor with acceptor centers on the surface are included. Since the mathematical treatments are similar for the two situations, a complete analysis will be given only for the p-type semiconductor, and the resulting equations of the other combination will be tabulated without derivations.

The surface donor centers introduce mobile electrons into the conduction band of the space charge region. On a p-type semiconductor

then the space charge region at the surface must become less p-type. However, the hole neutralization can proceed to the point where the surface becomes intrinsic, or even n-type. These changes, of course, depend on the bulk carrier concentration and the ionized surface donor concentration.

A criterion for these changes can be obtained by the fact that at the intrinsic plane,  $p(x) = n(x) = n_i$ . For a p-type semiconductor the bulk charge density variation is given by Equation (31a).

At the intrinsic plane, the sum of the mobile charge must be equal to zero and the particular value of diffusion potential,  $\mathbf{u_i}$ , is defined. That is

$$sinh (u_B' - u_i) = 0$$

The intrinsic diffusion potential can be related to the bulk properties of the semiconductor, since

$$u_i = u_B' = \ln (p_B/n_B)^{1/2}$$
 (49)

Equation (49) can be translated into more convenient form, since

$$u_{B}' = u_{i} = \ln \left( \frac{p_{B}}{p_{B}} - \frac{p_{B}}{n_{B}} \right)^{1/2} = \ln \left( \frac{p_{B}^{2}}{n_{i}^{2}} \right)^{1/2} = \ln \left( \frac{p_{B}}{n_{i}^{2}} \right)^{1/2}$$

Recall that  $n_i = (N_V N_C)^{1/2} \exp(-Eg/2 kT)$ 

Therefore

$$u_{B}' = u_{i} = \frac{Eg}{2 k T} + \ln \left\{ \frac{p_{B}}{N_{V}N_{C}} \right\}^{1/2}$$
 (50)

When the surface potential is equal to the intrinsic diffusion potential, then the outermost surface is just intrinsic.

Whether there is an inversion in the space charge region or just a depletion of majority carriers depends on the relationship between the bulk carrier concentration of the semiconductor and the ionized surface donor concentration.

In order to establish the various relationships it will be assumed that a constant ionized surface donor concentration is created on various p-type semiconductor substrates having widely different electrical conductivities. Three cases will be discussed in the following subsections. In Case 5 surface donors form a depletion layer on a highly doped p-type semiconductor, and the surface potential is small, such that

$$u_{s} \leq \ln \left(\frac{p_{B}}{n_{B}}\right)^{1/2} \tag{51}$$

There is no inversion of the space charge region, although the surface may attain an intrinsic condition. In Case 7 surface donors form an inversion layer on a moderately doped p-type semiconductor. There is an inversion in the space charge region, but at most

$$u_s = 2 \ln \left(\frac{p_B}{n_B}\right)^{1/2}$$

or in general

$$\ln \left(\frac{p_B}{n_B}\right)^{1/2} < u_s \leq 2 \ln \left(\frac{p_B}{n_B}\right)^{1/2} \tag{52}$$

In Case 9 surface donors form an inversion layer on nearly intrinsic, p-type semiconductor, and the surface potential is large, such that

$$u_{s} > 2 \ln \left(\frac{p_{B}}{n_{B}}\right)^{1/2} \tag{53}$$

There is an inversion in the space charge region. Each of these three subcases is discussed in considerably more detail.

# Case 5a. Surface Donors Form a Depletion Layer on a Highly Doped p-Type Semiconductor.

In this situation
$$u_{s} \leq \ln \left(\frac{p_{B}}{n_{B}}\right)^{1/2} \tag{51}$$

but the surface never becomes intrinsic or n-type.

# a) The Surface Potential, us.

Substitution of Equation (31a) into Poisson's Equation, Equation (12), and integration using the boundary conditions from Equations (13), (14) and (15) gives

$$\left(\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}\mathbf{x}}\right)^{2} = 4 \, \mathrm{L}_{\mathrm{m}} \left[ \left(N_{\mathrm{a}}\right) \, \mathrm{u}_{\mathrm{s}} + 2 \, \mathrm{n}_{\mathrm{i}} \left[ \cosh\left(\mathrm{u}_{\mathrm{s}} - \mathrm{u}_{\mathrm{B}}\right) - \cosh\left(\mathrm{u}_{\mathrm{B}}\right) \right] \right]$$
(54)

The following identities can be formed.

$$2 n_{i} \left\{ \cosh \left( u_{s} - u_{B}' \right) \right\} = 2 n_{i} \left\{ \cosh \left( u_{B}' - u_{s} \right) \right\}$$

$$= 2 n_{i} \left\{ \cosh u_{B}' \cosh u_{s} - \sinh u_{B}' \sinh u_{s} \right\}$$

$$= \left( p_{B} + n_{B} \right) \cosh u_{s} - \left( p_{B} - n_{B} \right) \sinh u_{s}$$

$$= p_{B} \left[ \cosh u_{s} - \sinh u_{s} \right] + n_{B} \left[ \cosh u_{s} + \sinh u_{s} \right]$$

$$= p_{B} \exp \left( -u_{s} \right) + n_{B} \exp \left( u_{s} \right)$$

In addition, since

$$n_{B} = p_{B} \left( \frac{n_{B}}{p_{B}} \right) = p_{B} \left( \frac{n_{B}}{p_{B}} \right)^{1/2}$$

$$= p_{B} \exp \left(-2 u_{B}'\right)$$

then substitution of these identities into Equation (54) gives

$$2 n_i \cosh(u_s - u_B') = p_B \exp(-u_s) + p_B \exp(-2 u_B' + u_s)$$
 (55)

Combine (54) and (55) and note that 2 n  $\cosh u_B' = (p_B + n_B)$ .

The result is

$$\left(\frac{du}{dx}\right)_{0}^{2} = 4L_{m} \left((N_{a}^{-}) u_{s} + p_{B} \exp(-u_{s}) + p_{B} \exp(-2 u_{B}^{+} + u_{s}) - (p_{B}^{+} + n_{B})\right)$$
(56)

Since

$$u_B' > u_s > 1$$

then

$$\exp (-2 u_B' + u_S) < \exp (-u_S') < < 1$$

For  $u_s = 3$ , then  $\exp(-u_s) = 0.05 <<1$ , which is a sufficient approximation. For an acceptor-doped semiconductor wherein  $u_B'>>1$ , then  $p_B = (N_a)$  and Equation (56) becomes

$$\left(\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}\mathbf{x}}\right)_{0}^{2} \simeq 4 \, \mathrm{L}_{\mathrm{m}} \, (\mathrm{N}_{\mathrm{a}}^{-}) \left\{\mathrm{u}_{\mathrm{s}} - 1\right\} \tag{57}$$

Now Equation (57) can be combined with the square of Equation (20) from Section A to give

$$4 L_{m}^{2} (\sigma_{a}^{+})^{2} = 4 L_{m} (N_{a}^{-}) \{u_{s} - 1\}$$

Therefore

$$u_{s} = \left\{ \left( \frac{L_{m}}{N_{a}} \right) \left( \sigma_{Q}^{+} \right)^{2} \right\} + 1$$
 (58)

and the surface potential is related to the ionized surface donor density and the ionized bulk acceptor density.

# Case 5b Surface Donors Form an Intrinsic Surface Layer on a Highly-Doped p-Type Semiconductor.

# a) The Surface Potential, us.

For the condition  $u_s \simeq u_B'$ , then  $\cosh(u_s - u_B') \simeq 1$  and Equation (54) becomes

$$\left(\frac{du}{dx}\right)_{0}^{2} = 4 L_{m} \left\{ (N_{a}^{-}) u_{s} + 2 n_{i} - (p_{B} + n_{B}^{-}) \right\}$$
 (59)

Since

$$2 n_i = 2 \sqrt{p_B n_B}$$

Furthermore since

$$n_B = p_B \exp(-2u_B')$$
 and  $n_B^{1/2} = p_B^{1/2} \exp(-u_B')$ 

Then

$$2n_{i} - (p_{B} + n_{B}) = -\left(p_{B}^{1/2} - n_{B}^{1/2}\right)^{2} = -p_{B}\left[1 - \exp(-u_{B}')\right]^{2} = -p_{B}(60)$$

The last approximation is valid if  $\exp(-u_B') << 1$ . Combine Equations (59) and (60)

$$\left(\frac{du}{dx}\right)_{0}^{2} = 4 L_{m} \left\{ (N_{a}^{-}) u_{s} - p_{B} \right\}$$
Since  $p_{B} = N_{a}^{-} + n_{B} \cong N_{a}^{-}$ , then
$$\left(\frac{du}{dx}\right)_{0}^{2} = 4 L_{m} \left\{ u_{s} - 1 \right\} (N_{a}^{-})$$
(57)

Therefore for Cases 5a and 5b Equation (57) was obtained in each case for  $u_B^+ \ge u_S^- \ge 3$  and the relationship between surface potential and surface charge density is given by Equation (58). The approximation requires only that  $\exp(-u_S^-) < 1$ .

# a) The Diffusion Potential, u(x).

After the formulation of the relationship between the surface potential and the surface ion concentration, the diffusion potential variation inside the semiconductor can be formulated. By removing the boundary condition defined by Equation (15) then Equation (56) can be rewritten

$$\left(\frac{du}{dx}\right)^{2} = 4 L_{m} \left\{ (N_{a}^{-}) u + p_{B} \exp(-u) + p_{B} \exp(-2 u_{B}^{-} + u) - (p_{B}^{-} + n_{B}^{-}) \right\}$$
(56a)

In the neighborhood of x = 0, where  $u_B' \ge u_s$ , and both are much larger than unity, then Equation (56a) reduces to

$$\left(\frac{du}{dx}\right)^2 = 4 L_m \left(N_a^-\right) \left[u-1\right] \tag{57a}$$

Taking the square root with the negative sign, as was done in Equation (19) the result is

$$\left(\frac{du}{dx}\right) = -2 \left[L_{m}\left(N_{a}\right)\right]^{1/2} \left(u-1\right)^{1/2}$$
 (61)

Since Equation (61) is applicable for the neighborhood of x = 0,

it can be integrated for small values of x extending from the surface.

$$\int_{u_s}^{u} (u-1)^{-1/2} d(u-1) = -2 \left[L_m N_a^{-1}\right]^{1/2} x$$

Therefore

$$(u-1)^{1/2} = (u_s-1)^{1/2} - [L_m(N_a^-)]^{1/2} \times$$
 (62)

For u (x) in the neighborhood of unity, as x extends into the interior of the solid, Equation (56a) has to be reevaluated and simplified again before performing the integration. The significant term then is  $p_B \exp(-u)$ . Equation (56a) then becomes

$$\left(\frac{du}{dx}\right)^2 = 4 L_m p_B \exp(-u)$$
 (63)

Again, taking the square root with the negative sign gives

$$\left(\frac{du}{dx}\right) = -2 \left(L_{m} p_{B}\right)^{1/2} \exp\left(-u/2\right)$$
 (63a)

In order to determine a boundary condition at which these two cases merge, consider that the slopes of the diffusion potential must be equal when calculated from each set of assumptions. Therefore Equation (57a) must be equal to Equation (63) at a particular value of  $u=u_2$ , and this value can be determined,

$$4 L_{m} (N_{a}) (u_{2} - 1) = 4 L_{m} (N_{a}) \exp(-u_{2})$$

Therefore  $\mathbf{u}_2$  is the root of the equation

$$u_2 = 1 + \exp(-u_2)$$
 $u_2 = 1.28$  (64)

The value of  $x_2$  corresponding to this value of  $u_2$  then is obtained from Equation (62) and is

$$x_{2} = \frac{\sqrt{u_{s} - 1} - 0.53}{\sqrt{L_{m} (N_{a})}}$$
 (65)

The integration of Equation (63a) now can be completed.

$$\int_{u=1.28}^{u=u} \exp(u/2) d(u/2) = -(L_m p_B)^{1/2} x + \sqrt{u_s-1} - 0.53$$

That is

$$\exp (u/2) = \exp .64 - (L_m p_B)^{1/2} x + \sqrt{u_s - 1} - 0.53$$

or

$$u = 2 \ln \left\{ 1.37 - (L_{m} p_{B})^{1/2} x + \sqrt{u_{s} - 1} \right\}$$
 (66)

For values of x approaching infinity, such that u(x) is very small and approaching zero, then the exponential factor in Equation (56a) can be expanded in series form.

$$p_{B} \exp (-u) \cong p_{B} (1 - u + \frac{u^{2}}{2} - ...)$$

and

$$n_{B} \exp u = n_{B} (1 + u + \frac{u^{2}}{2} + ...)$$

By substituting the above relationships into Equation (56a) one obtains

$$\left(\frac{du}{dx}\right)^{2} = 4 L_{m} \left\{ (N_{a}^{-}) u - (p_{B} - n_{B}) u + (p_{B} + n_{B}) + \frac{1}{2} (p_{B} + n_{B}) u^{2} - (p_{B} + n_{B}) \right\}$$

$$= 4 L_{m} \left\{ \frac{1}{2} (p_{B} + n_{B}) u^{2} \right\}$$

$$(67)$$

Therefore, taking the square root with the negative sign, as before, since u decreases as x increases.

$$\left(\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}\mathbf{x}}\right) = -\left[2 L_{\mathrm{m}} \left(p_{\mathrm{B}} + n_{\mathrm{B}}\right)\right]^{1/2} \mathbf{u} \tag{68}$$

The boundary condition between these last two cases can be approximated by equating Equations (63) and (67). This shows that

$$2 = u_3^2 \exp u_3$$

From which it follows that

$$u_3 = 0.90$$

When this value for  $u_3$  is substituted into Equation (66) the corresponding value of  $x_3$  is found to be

? 
$$x_3 = \frac{1.50 + \sqrt{u_s - 1}}{\sqrt{L_m p_B}}$$
 (69)

Equation (68) now can be integrated, assuming that  $p_B > n_B$ .

$$\int_{u_3}^{u} \frac{du}{u} = -\sqrt{2 L_m p_B} \int_{x_3}^{x} dx$$

Therefore

$$\ln u/u_3 = -\sqrt{2 L_m p_B} \left\{ x - \frac{1.5 + \sqrt{u_s - 1}}{\sqrt{L_m p_B}} \right\}$$

or

$$u(x) = 0.9 \exp \left(-x \sqrt{2 L_m p_B} + 2.121 + \sqrt{2} \sqrt{u_s - 1}\right) (70)$$

In summary in this highly doped extrinsic semiconductor, the diffusion potential in the semiconductor can be approximately represented by Equations (62), (66) and (70) in increasing magnitude of x.

# Case 6. Surface Acceptors Form Depletion-Inversion Layer on a Highly-Doped n-Type Semiconductor.

As has already been observed in Cases 1 and 2, and Cases 3 and 4, there is a symmetrical relationship between the results which are obtained when a p-type semiconductor is replaced with an n-type semiconductor, and surface donors are replaced with

surface acceptors. The surface potential and bulk diffusion potential can be expressed with the equations already derived by changing from an electron energy reference to a hole energy reference, and making the appropriate changes in the majority carrier and surface ion designations.

# Case 7. Surface Donors Form an Inversion Layer on a Moderately-Doped p-Type Semiconductor.

In this case we specify that the adsorbed ion is such that

$$\ln \left(\frac{p_B}{n_B}\right)^{1/2} < u_S \le 2 \ln \left(\frac{p_B}{n_B}\right)^{1/2}$$
 (52)

The surface is inverted but the magnitude of the inversion is moderate, and does not exceed the magnitude of the bulk diffusion potential. The bulk diffusion potential,  $u_B^{\phantom{B}}$ , in this case must be equal to or greater than 3 units of kT, since results obtained from Case 5 are to be used in this derivation

# a) The Surface Potential, u<sub>s</sub>.

To formulate u as a function of  $\sigma_{\square}^+$  the following approximation can be used.

$$u_s = 2 u_B' = \ln \left(\frac{p_B}{n_B}\right)$$

When this substitution is made into Equation (54) it reduces immediately to

$$\left(\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}\mathbf{x}}\right)^{2} = 4 L_{\mathrm{m}} (N_{\mathrm{a}}) u_{\mathrm{s}} \tag{71}$$

Combine Equation (71) with the square of Equation (20)

$$u_{s} = \left\{ \frac{L_{m}}{N_{a}} - \left[ \sigma_{D}^{+} \right]^{2} \right\}$$
 (72)

This equation has been derived previously by Aigrain and Dugas,  $^3$  by Hauffe and Engell,  $^1$  and by Weiss  $^4$  using a different model and

different boundary conditions.

## b) The Diffusion Potential, u(x).

For u(x) as function of x, the following regions can be differentiated. In the neighborhood of x = 0, from Equation (71), but eliminating the boundary condition from Equation (15):

$$\left(\frac{du}{dx}\right) = -2 \left(L_{m} N_{a}^{-1}\right)^{1/2} u$$
 (73)

Integration of Equation (73) using the boundary conditions of Equation (15) and (72) gives

$$u^{1/2} = u_s^{1/2} - \sqrt{L_m N_a} \times = \sqrt{L_m N_a} \left( \frac{\sigma_C^+}{N_a^-} - x \right)$$
 (74)

This is the well known Mott - Schottky 11 region. Garrett and Brattain 5 have discussed Equation (74), but mistakenly state that there is not yet an inversion in the space charge region.

This equation relating diffusion potential to position should be valid until the diffusion potential approaches the intrinsic plane. From the intrinsic plane on into the interior of the semiconductor, the concepts developed in conjunction with Case 5 should be applicable. The point at which Equation (74) should be replaced with another expression can be estimated by letting  $u = u_{\hat{i}}$  in Equation (74). This can be solved to show that

$$x_{i} = \frac{\sqrt{u_{s} - \sqrt{u_{B}^{'}}}}{\sqrt{L_{m}N_{a}^{-}}} \simeq \frac{\left(1 - \frac{1}{\sqrt{2}}\right)\sqrt{u_{s}}}{\sqrt{L_{m}N_{a}^{-}}}$$
(75)

This point now can be used as a boundary condition in the integration of Equation (61). The result of this integration over small intermediate ranges of x wherein u is close to u, and substitution shows that

$$\sqrt{u-1} = \sqrt{u_s-1} + \left(1 - \frac{1}{\sqrt{2}}\right)\sqrt{u_s} - x/L_m p_B \tag{76}$$

This equation is similar to Equation (62), differing only in the integration constant. Equation (76) then should be valid until  $u_2 = 1.28$ . However, this will no longer occur at the same value of  $x_2$ . The new boundary condition must be evaluated from Equation (76) for  $u_2 = 1.28$ . The result is

$$x_{2}' = \frac{\sqrt{u_{s} - 1} + 0.293 \sqrt{u_{s}} - 0.53}{\sqrt{L_{m} p_{B}}}$$
 (77)

For larger intermediate values of x, the variation of u can be obtained by integrating Equation (63a) using Equation (77) as a boundary condition. The result is

$$\exp(u/2) = 3.07 - x \sqrt{L_m p_B} + \sqrt{u_S - 1} + 0.293 u_S$$
 (78)

This relationship is valid until  $u_3 = 0.90$ , and the new value of  $x_3$  defined for this value of  $u_3$  can be found from Equation (78). The re-

sult is 
$$x_{3}' = \frac{1.50 + \sqrt{u_{s} - 1} + 0.293 \sqrt{u_{s}}}{\sqrt{L_{m} p_{B}}}$$
 (79)

This boundary condition now can be used to integrate Equation (68), for large values of x. The result is

$$u = 0.90 \exp(-x\sqrt{2} L_{m}p_{B} + 2.121 + \sqrt{2} \sqrt{u_{s}-1} + 0.414 \sqrt{u_{s}})$$
 (80)

Equation (80) is valid for all values of x greater than that defined by Equation (79) and u goes to zero as x approaches infinity as required by the boundary condition defined in Equation (13).

# Case 8. Surface Acceptors Form an Inversion Layer on a Moderately Doped n-Type Semiconductor.

The equation derived under Case 7 also can be used in this case by changing the designations as was done in Cases 2, 4 and 6.

# Case 9. Surface Donors Form an Inversion Layer on a Nearly In-

### trinsic p-Type Semiconductor.

In this case the surface potential,  $\mathbf{u}_{_{\mathbf{S}}}$  , is greater than 2  $\mathbf{u}_{_{\dot{\mathbf{I}}}}$  . That is

$$u_{s} > \ln\left(\frac{p_{B}}{n_{B}}\right) \tag{53}$$

By removing the boundary condition defined by Equation (15), then Equation (54) can be rewritten and transformed using a relation similar to Equation (34). The result is

$$\left(\frac{du}{dx}\right)^{2} = 4 L_{m} \left( \left( N_{a} \right) u + 4 n_{i} \sinh \left( \frac{u}{2} - u_{B} \right) \sinh u / 2 \right)$$

Furthermore since

$$\sinh (u/2 - u_B') = \exp (u_B') \sinh (u/2) - \exp (-\frac{u}{2}) (\sinh u_B')$$

and

$$2 n_i \sinh u_B' = p_B - n_B = (N_a)$$

then

$$\left(\frac{du}{dx}\right)^2 = 4 L_m \left(N_a^-\right) \left[u-1 + \exp(-u)\right] + 4 n_i \exp(-u_B^-) \sinh^2(u/2) \right\}$$
 (81)  
Since

 $n_i \exp(-u_R^i) = n_R^i$ 

$$(N_a) = p_B - n_B$$

$$\left(\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}\mathbf{x}}\right)^{2} = 4 L_{\mathrm{m}} \left\{ p_{\mathrm{B}} \left[ \mathbf{u} - 1 + \exp\left(-\mathbf{u}\right) \right] + n_{\mathrm{B}} \left[ \exp\left(\mathbf{u}\right) - \mathbf{u} - 1 \right] \right\}$$
(82)

# a) The Surface Potential, us.

Equation (82) can be evaluated at the surface using the boundary condition defined by Equation (15) with the further restriction that  $\exp(u_s) >> u_s$ , and therefore  $\exp(-u_s) << 1$ . By using Equation (30a) it follows directly that

$$\left(\frac{du}{dx}\right)_{0}^{2} = 4 L_{m} \left\{ p_{B} \left(u_{s} - 1\right) + p_{B} \exp\left(\pm 2 u_{B}' + u_{s}\right) \right\}$$
(83)

By inspecting Equation (83) and realizing that  $u_s \gg 2$   $u_B$  in this case, then the second term in the right-hand side of this equation is dominating. This approximation is valid when

$$n_B \exp (u_S) = \gamma p_B (u_S - 1)$$

or

$$u_s = 2 u_B' + ln [\gamma (u_s - 1)]$$
 (84)

 $\gamma$  = 20, is sufficient for most experimental cases.

With the simplification then Equation (83) becomes

$$\left(\frac{du}{dx}\right)_{0}^{2} = 4 L_{m} n_{B} \exp\left(u_{S}\right)$$
 (85)

When combined with the square of Equation (20), the final result is

$$u_{s} = \ln \left\{ \frac{L_{m}}{n_{B}} \left( \sigma_{D}^{+} \right)^{2} \right\} = 2 u_{B}^{+} \ln \left\{ \frac{L_{m}}{p_{B}} \left( \sigma_{D}^{+} \right)^{2} \right\}$$
(86)

Now if the two terms in Equation (83) are approximately of the same order of magnitude the result becomes

$$\left(\frac{du}{dx}\right)_{0}^{2} = 4 L_{m} p_{B} \left\{ \exp \left[ \ln \left( u_{S} - 1 \right) + u_{S} - 2 u_{B}^{*} \right] \right\}$$
(87)

When this result is combined with the square of Equation (20), the result is

$$u_{s} + \ln (u_{s} - 1) - \ln (\frac{p_{B}}{n_{B}}) = \ln \left\{ \frac{L_{m}}{p_{B}} (\sigma_{B}^{+})^{2} \right\}$$

$$u_{s} + \ln (u_{s} - 1) = \ln \left\{ \frac{L_{m}}{n_{B}} (\sigma_{B}^{+})^{2} \right\} = 2 u_{B}^{+} \ln \left\{ \frac{L_{m}}{p_{B}} (\sigma_{B}^{+})^{2} \right\}$$
(88)

Either Equation (86) or Equation (88) can be used to relate the surface potential to the surface charge and bulk carrier concentration of the nearly intrinsic p-type semiconductor.

#### b) The Diffusion Potential, u(x).

The diffusion potential as function of distance can be divided

into regions. In the neighborhood of x = 0, for large values of  $u_s$ , Equation (85) can be reformulated as

$$\left(\frac{du}{dx}\right) = -2 \left(L_{m} n_{B}\right)^{1/2} \exp\left(u/2\right) = -2 \sqrt{L_{m} p_{B}} \exp\left(-u_{B}\right) \exp\left(u/2\right)$$
 (89)

Integration from the surface of the semiconductor into the interior gives

$$\int_{u_{s}}^{u} \exp(-u/2) du = -2 (L_{m}n_{B})^{1/2} x = -2 x \sqrt{L_{m}p_{B}} \exp(-u_{B})$$

or

$$u = -2 \ln \left\{ \exp \left(-u_s/2\right) + x \left(L_m n_B\right)^{1/2} \right\}$$
 (41)

This equation is equal to Equation (41) which was derived for Case 3, an accumulation layer on an n-type semiconductor.

When it is realized that now the substrate is a p-type semiconductor, then this equation can be rearranged to the form

$$u = -2 \ln \left\{ \exp \left(-u_{s}/2\right) + x \sqrt{L_{m}p_{B}} \exp \left(-u_{B}\right) \right\}$$
or
$$u = 2 u_{B} - 2 \ln \left\{ \exp \left(u_{B} - u_{s}/2\right) + x \sqrt{L_{m}p_{B}} \right\}$$
(90)

This relationship is valid as long as  $u_s > 2 u_B'$ . When  $u_s = 2 u_B'$ , then a value of  $x_1$  can be evaluated, which is

$$x_{1} = \frac{1 - \exp(u_{B} - u_{s}/2)}{\sqrt{L_{m} p_{B}}}$$
 (91)

A more precise boundary between the limits of applicability can be found by equating Equations (89) and (73), and obtaining the root  $u_1$  at which these two slopes are equal. The result is

$$u_1 = \exp(-2 u_B) \exp u_1 \tag{92}$$

This boundary condition then depends directly on the bulk diffusion potential,  $u_B$ . The root from Equation (92) then can be substituted into Equation (90) in order to evaluate  $x_q$  more precisely. This re-

sult then is

$$x_{1} = \frac{\exp (u_{B} - u_{1}/2) - \exp (u_{B} - u_{S}/2)}{\sqrt{L_{m} p_{B}}}$$
(93)

or

$$x_1 = \sqrt{\frac{1}{u_1}} - \exp(u_B - u_s/2)$$

$$\sqrt{L_m p_B}$$
(93a)

This case then can be superimposed on Case 7 and Case 5 for the situation wherein  $u_B > 1.5$ . The variation of u as a function of x is expressed by Equation (90) until the value of  $x_1$  is reached.

# Case 10. Surface Acceptors Form an Inversion Layer on a Nearly Intrinsic n-Type Semiconductor.

The relationships obtained from Case 9 can be applied symmetrically to the reciprocal situation as was done in Cases 2, 4, 6 and 8.

#### Conclusion.

In this work the surface potential and the diffusion potential have been related to the bulk diffusion potential and the surface ion concentration for all combinations of surface charge and types of semiconductors.

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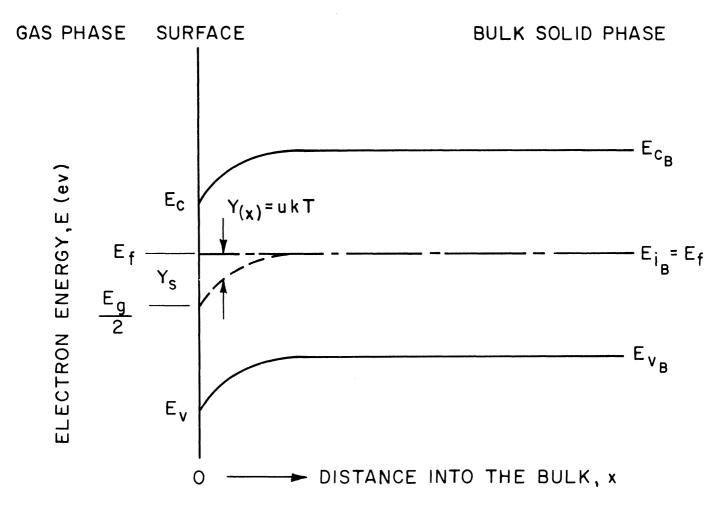


Figure 1. Electron potential energy diagram for donors on the surface of an intrinsic semiconductor. (Not to scale.)

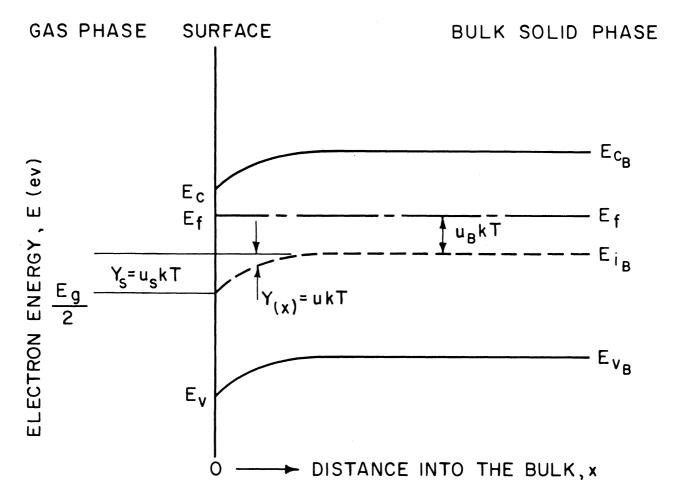


Figure 2. Electron potential energy diagram for donors on the surface of an n-type semiconductor. (Not to scale.)

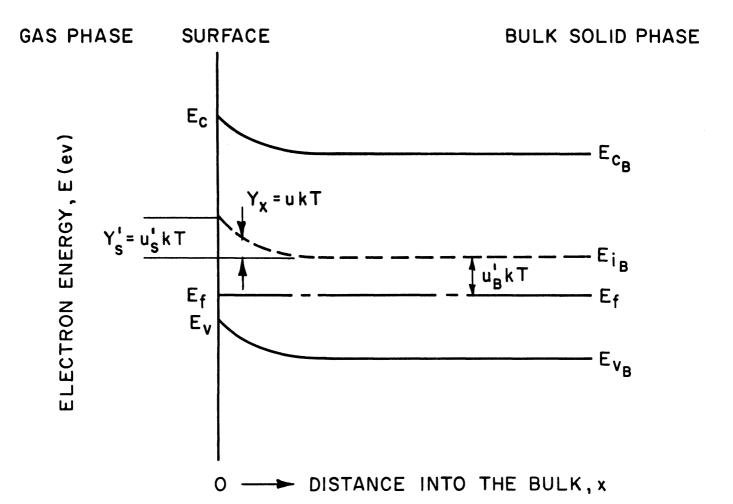


Figure 3. Electron potential energy diagram for acceptors on the surface of a p-type semiconductor. (Not to scale.)

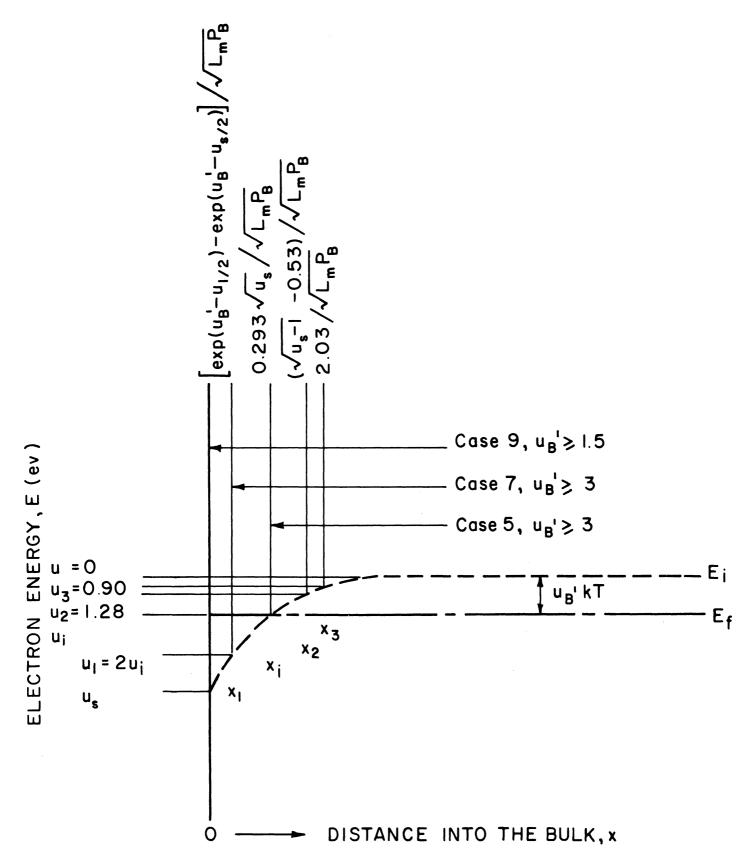


Figure 4. Variation of mid-band electron potential energy position for a depletion-inversion layer created by donors on the surface of a p-type semiconductor. (Not to scale.)