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An extended and unified solution for the semiconductor surface problem at equilibrium

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An equilibrium solution is presented for the semiconductor surface in terms of the potential, electric field, charge density, and change in mobile-carrier concentrations throughout the semiconductor as a function of the surface potential and bulk doping. These results are an extension of the work initiated by R. H. Kingston and S. F. Neustadter [J. Appl. Phys. **26**, 718 (1955)]; and extended by C. E. Young [J. Appl. Phys. **32**, 329 (1961)]. The present results cover a wider range of all the parameters involved in the problem; also, through quantities chosen for normalization and through choice of origin, the present results remove a considerable redundancy existing in the previous data. Finally, the identity of the equilibrium surface problem and the equilibrium step-junction problem is demonstrated and explained.

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A recent analysis has provided a general solution for step junctions at equilibrium.[1] The same solution applies to the semiconductor surface problem (i.e., to the semiconductor portion of an MIS capacitor), a Schottky junction, or a heterojunction, as we show here. The present results subsume and extend those of Kingston and Neustadter[2] and Young,[3] while diminishing substantially the redundancy present in the earlier results. It is emphasized that like the above-mentioned analyses, the present formulation is valid only under equilibrium.

From Ref. 1 we have for a step junction

$$\frac{x}{L_{\mathrm{De}}} = \frac{1}{\sqrt{2}} \int_{W}^{W_J} \left(\frac{e^{U_{20}} + e^{-U_{20}}}{e^{U_{20}}(e^{-W'} - 1 + W') + e^{-U_{20}}(e^{+W'} - 1 - W')} \right)^{1/2} dW'. \quad (1)$$

Here U_{20} is the normalized bulk potential on the right-hand side of the junction, x the distance to the right of the junction, L_{De} the extrinsic Debye length, $W = U_{20} - U$, where the normalized potential U is defined by the relations $n = n_i \exp(U)$, [or $p = n_i \exp(-U)$], and $W_J = U_{20} - U_J$, where U_J is the normalized potential at the junction.

The conversion from potential U to potential W amounts to changing the potential reference from the Fermi level to the bulk potential, and reversing algebraic sign. Apropos the latter point, note that (for example) on the N side of a symmetric junction at equilibrium, U goes from the positive value U_{20} in the bulk to zero at the junction, while W goes from zero in the bulk to U_{20} at the junction.

In the surface problem it is pertinent to talk in terms of the surface instead of the junction. Therefore, let us place the surface of the present problem at the position of junction in the previous problem, so that $W_J \equiv W_S$. It follows, therefore, that W_S is the total band bending in the sample. Equation (1) is converted from the junction problem to the surface problem simply by substituting W_S for W_J as the upper limit of the integral. The potential profiles found earlier[1] apply equally here, and are presented over an extended range as in Fig. 1.

To get the field profile we differentiate Eq. (1) and obtain

$$\left| \frac{dW}{d(x/L_{\mathrm{De}})} \right| = (\sqrt{2}) \left(\frac{e^{U_{20}}(e^{-W} - 1 + W) + e^{-U_{20}}(e^{W} - 1 - W)}{e^{U_{20}} + e^{-U_{20}}} \right)^{1/2}. \quad (2)$$

The sign to be attached is clear from the problem addressed. These curves are presented in Fig. 2.

Adding algebraically the densities of all of the fixed and mobile charges present at an arbitrary point, we obtain the net charge density,

$$|\rho_{\mathrm{net}}| = 2qn_i |\sinh U_{20} - \sinh U|$$
$$= 2qn_i |\sinh U_{20} - \sinh (U_{20} - W)|. \quad (3)$$

It is convenient to express this net charge density as a fraction of the total density of mobile charge present in the bulk, $\rho_0 = q(n+p)$, yielding

$$\left| \frac{\rho_{\mathrm{net}}}{\rho_0} \right| = \left| \frac{\sinh U_{20} - \sinh (U_{20} - W)}{\cosh U_{20}} \right|. \quad (4)$$

This function is plotted in Fig. 3.

Comparing present results with the earlier results[2,3] is facilitated by computing the number of charges per unit area near the semiconductor surface in the form of excess holes and electrons for various values of surface potential. This

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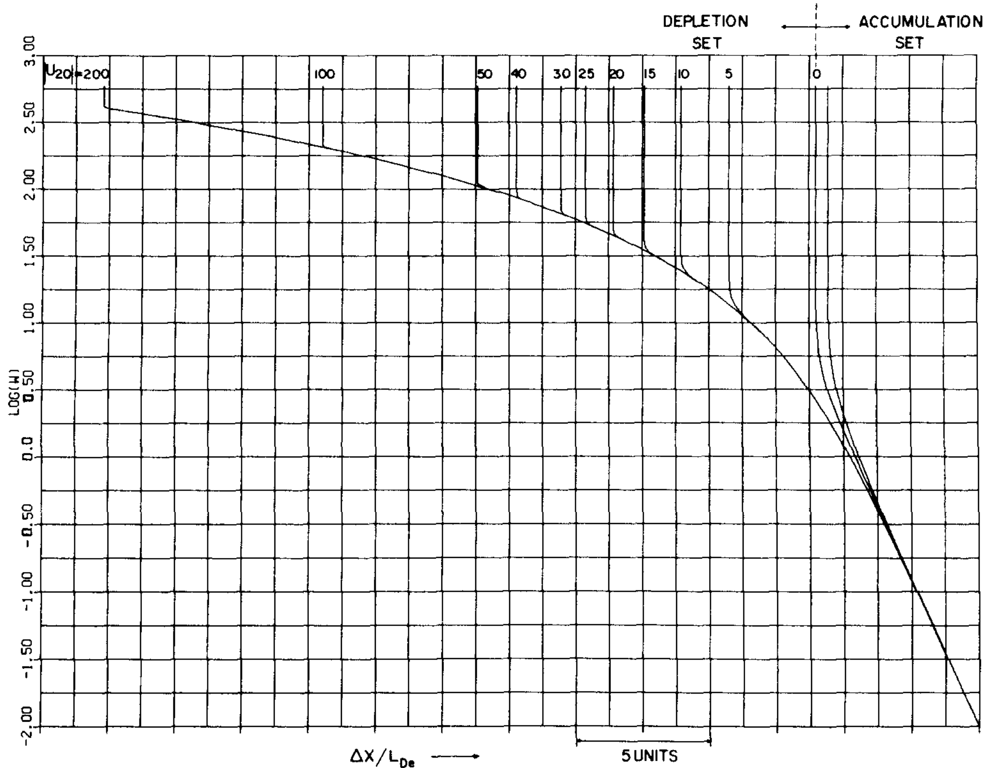

FIG. 1. $W = (U_{20} - U)$ vs normalized distance, with $|U_{20}|$ as a parameter for the depletion set.

density can be written for holes as

$$\Delta N_p = n_i \int_0^\infty (e^{-U} - e^{-U_{20}})\, dx, \tag{5}$$

where the origin of x is placed at the surface. Similarly, for electrons,

$$\Delta N_n = n_i \int_0^\infty (e^{U} - e^{U_{20}})\, dx. \tag{6}$$

It is convenient to use for normalization the number of carriers of a given type present in the bulk in a layer one extrinsic Debye length thick, or
$\Delta N_{p0} = L_{\mathrm{De}} n_i \exp(-U_{20})$, and $\Delta N_{n0} = L_{\mathrm{De}} n_i \exp(U_{20})$.
The magnitudes of the resulting ratios are

$$\left| \frac{\Delta N_p}{\Delta N_{p0}} \right| = \int_0^\infty (e^{W} - 1) \frac{dx}{L_{\mathrm{De}}}, \tag{7}$$

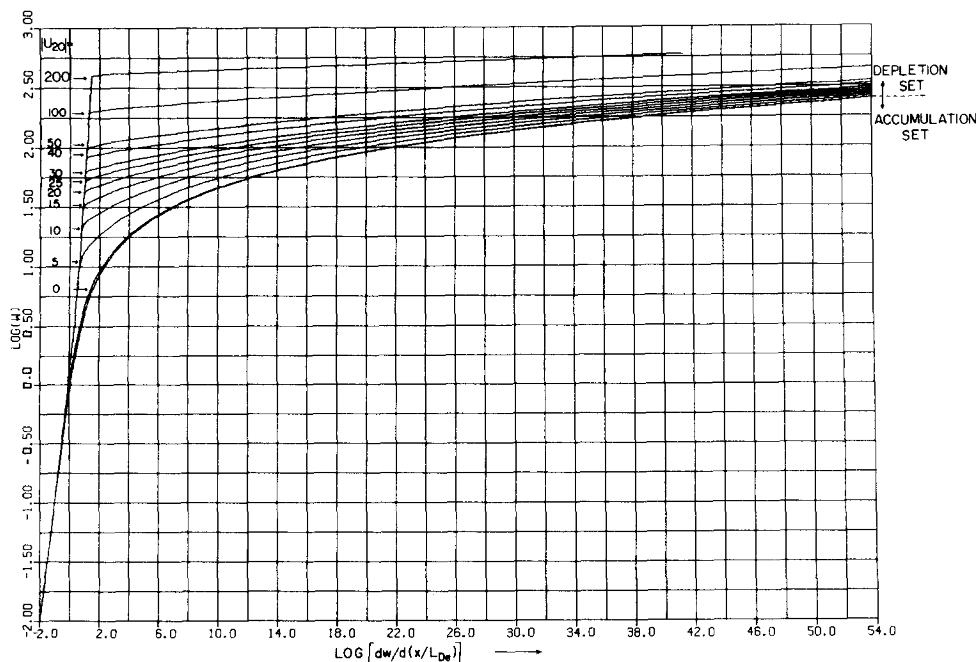

FIG. 2. Normalized electric field vs W, with $|U_{20}|$ as a parameter for the depletion set.

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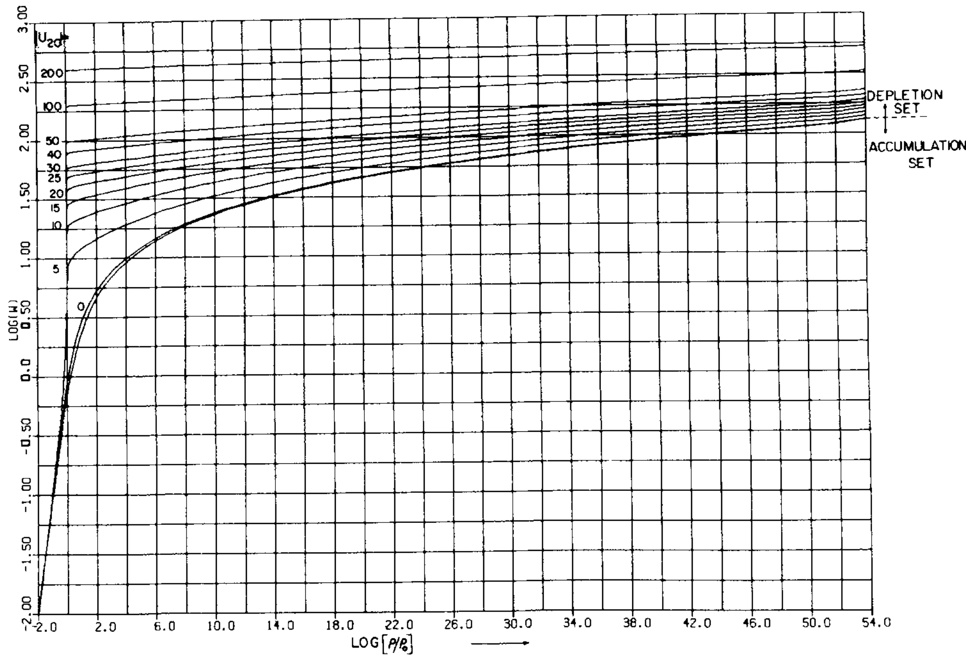

FIG. 3. Normalized charge density vs W, with $|U_{20}|$ as a parameter for the depletion set.

and

$$\left| \frac{\Delta N_n}{\Delta N_{n0}} \right| = \int_0^\infty (1 - e^{-W}) \frac{dx}{L_{De}}. \qquad (8) \tag{8}$$

Substituting the value of dx/L_{De} taken from Eq. (2) and altering the limits appropriately, we obtain

$$\left| \frac{\Delta N_p}{\Delta N_{p0}} \right| = \frac{1}{\sqrt{2}} \int_0^{W_S} \left(\frac{e^{U_{20}} + e^{-U_{20}}}{e^{U_{20}}(e^{-W} - 1 + W) + e^{-U_{20}}(e^{W} - 1 - W)} \right)^{1/2} (e^{W} - 1)\, dW, \tag{9}$$

and

$$\left| \frac{\Delta N_n}{\Delta N_{n0}} \right| = \frac{1}{\sqrt{2}} \int_0^{W_S} \left(\frac{e^{U_{20}} + e^{-U_{20}}}{e^{U_{20}}(e^{-W} - 1 + W) + e^{-U_{20}}(e^{W} - 1 - W)} \right)^{1/2} (1 - e^{-W})\, dW. \tag{10}$$

For each value of the parameter U_{20} selected, one can generate a curve representing the normalized number of excess carriers per unit area obtained by integrating from a point where the potential is W to a point deep in the bulk. Qualitatively there can be two physical situations: (1) majority carriers near the surface experience density elevation and simultaneously minority carriers experience density depression; (2) minority carriers near the surface experience density elevation and majority carriers experience density depression. Terms such as *accumulation*, *enhancement*, and *depletion* have all been preempted with specific meanings entrenched through long usage. It seems imprudent to tamper with those well-established definitions and so the generic terms *elevation* and *depression* are introduced to denote an obvious condition with respect to the density of either carrier type. Equation (9) has been derived for holes; for positive W it corresponds to density elevation, while for negative W it corresponds to density depression; Eq. (10) has been derived for electrons, but contrary to Eq. (9) for positive W it corresponds to density depression, while for negative W it corresponds to density elevation.

Thus far we have distinctly associated Eq. (9) with holes and Eq. (10) with electrons. However, because of the hole-electron symmetry in the problem as formulated, we observe that one equation transforms into another by simply changing the signs of both W and U_{20} simultaneously. Physically this implies that we can infer the results for both holes and electrons for density elevation from Eq. (9) by restricting ourselves to positive W, and for density depression from Eq. (10), again, be restricting to positive W.

Thus Fig. 4, which has been plotted from Eq. (9) for positive W, describes density elevation of *either* carrier type. It should be noted that Fig. 4 was generated while employing proper signs for U_{20}. However, in the figure these signs have been dropped in view of the dual utility of these curves. It represents *carrier density elevation*. Similarly Fig. 5 has been generated from Eq. (10) for positive W, finally depicting only $|U_{20}|$ as a parameter and representing *carrier density depression*.

In Fig. 4, the curve labeled $|U_{20}| = 0$ divides two cases. For the curves labeled "depletion set," the carrier whose density elevation is being examined is a minority carrier, and the action of the fixed ionic charge that is present causes the substantial dispersion of the curves. The "accumulation set"

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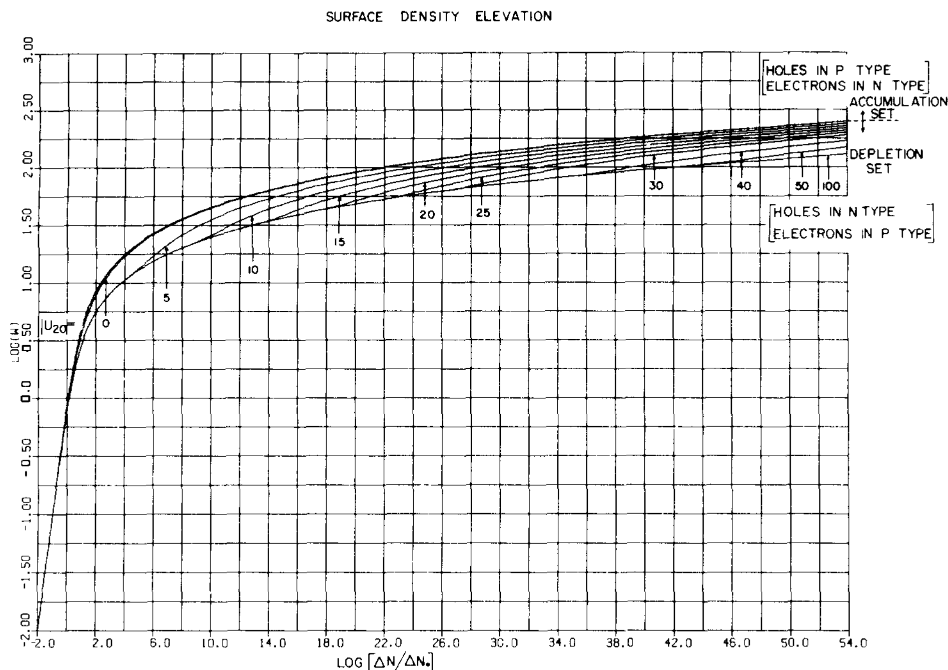

FIG. 4. Normalized excess areal density elevation of carriers vs W, with $|U_{20}|$ as a parameter for the depletion set.

is a single curve very near the $|U_{20}| = 0$ curve and represents majority-carrier-density elevation. Since these majority carriers completely mask the fixed charges in density, this set is virtually independent of $|U_{20}|$.

Similarly, in Fig. 5 also the curve labeled $|U_{20}| = 0$ divides two cases. The depletion set presents the case where fixed ionic charges dominate the behavior, and it is the density of majority carriers that is being depressed. The curve labeled accumulation set describes the depression of minority-carrier density that accompanies majority-carrier accounting for its slight dependence on $|U_{20}|$. Thus Figs. 4 and 5, each with two sets, cover all of the possibilities that exist.

Note that as one goes far away from the surface ($W \ll 1$), all curves merge removing all doping dependences. Note also the shapes of the curves in the regime where W is fairly large. It can be observed that the depletion sets maintain their distinctive "stiffness" (as opposed to the accumulation set) for values of $W \leqslant 2|U_{20}|$. Beyond this point, they acquire the general character of the accumulation set. This gives

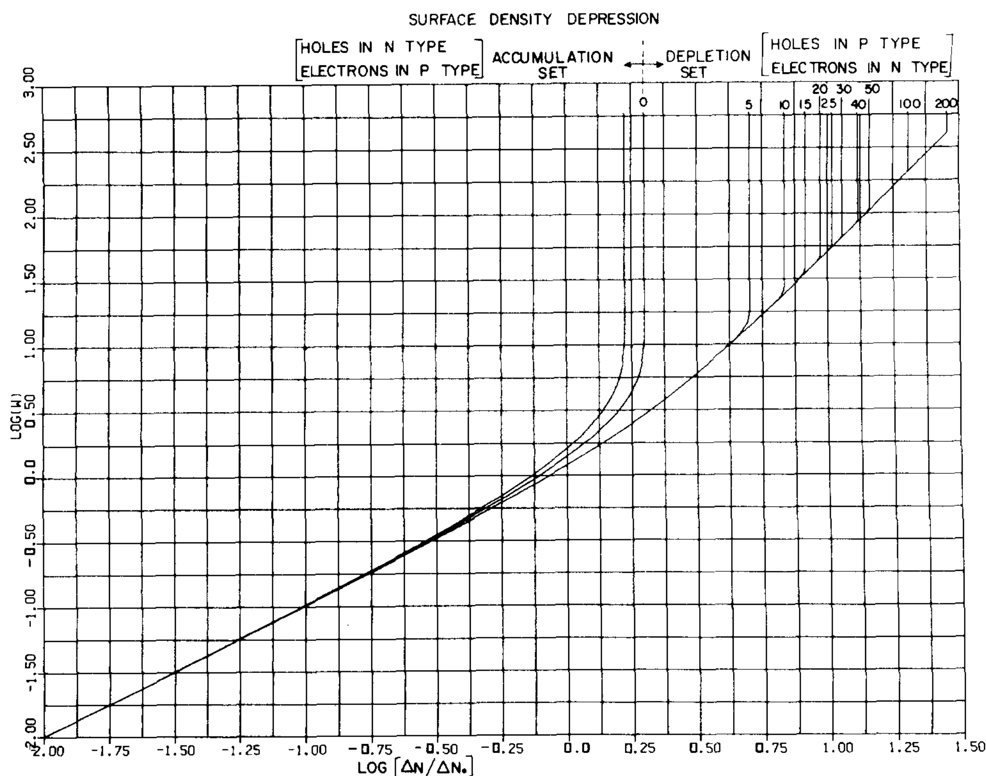

FIG. 5. Normalized excess areal density depression of carriers vs W, with $|U_{20}|$ as a parameter for the depletion set.

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added significance to $W = 2|U_{20}|$, which is conventionally referred to as the point of "onset of strong inversion." Beyond this point, the mobile carriers "take over" and the depletion set tends to follow the trend of the accumulation set.

DETAILED DERIVATION FOR LIMITING CASES

Case I: $W \leqslant 10^{-1}$

In this region for both accumulation and depletion sets, all the variables have an exceptionally simple dependence on W, i.e.,

$$\left|\frac{dW}{d(x/L_{De})}\right| = \left|\frac{\rho_{net}}{\rho_0}\right| = \left|\frac{\Delta N}{\Delta N_0}\right|_{elevation} = \left|\frac{\Delta N}{\Delta N_0}\right|_{depression} = W. \quad (11)$$

Hence, we have plotted all figures originating at $W = 10^{-2}$. Also in this regime from Ref. 1,

$$\frac{\Delta x}{L_{De}} = (\ln W_1 - \ln W_2), \quad (12)$$

which equals the separation between two points where the potential W attains the values W_1 and W_2.

Case II: $W \geqslant 10$, $U_{20} > 5$

Accumulation set

$$\Delta x/L_{De} = (\sqrt{2})[\exp(-\tfrac{1}{2}W_2) - \exp(-\tfrac{1}{2}W_1)], \quad W_1 > W_2, \quad (13)$$

$$\left|\frac{dW}{dx/L_{De}}\right| = (\sqrt{2})\exp(\tfrac{1}{2}W), \quad (14)$$

$$|\rho_{net}/\rho_0| = \exp(W) - 1. \quad (15)$$

For majority-carrier density elevation we have (Fig. 4)

$$\left|\frac{\Delta N}{\Delta N_0}\right|_{W=W_1} - \left|\frac{\Delta N}{\Delta N_0}\right|_{W=W_2} = (\sqrt{2})[\exp(\tfrac{1}{2}W_1) - \exp(\tfrac{1}{2}W_2)], \quad W_1 > W_2. \quad (16)$$

For minority-carrier density depression we have (Fig. 5)

$$\left|\frac{\Delta N}{\Delta N_0}\right|_{W=W_1} - \left|\frac{\Delta N}{\Delta N_0}\right|_{W=W_2} = (\sqrt{2})[\exp(-\tfrac{1}{2}W_2) - \exp(-\tfrac{1}{2}W_1)], \quad W_1 > W_2. \quad (17)$$

Depletion set

$$\frac{\Delta x}{L_{De}} = (\sqrt{2})[\sqrt{(W_1 - 1)} - \sqrt{(W_2 - 1)}], \quad W_2 < W_1 < |2U_{20}|, \quad (18)$$

$$\frac{\Delta x}{L_{De}} = (\sqrt{2})e^{U_{20}}[(\exp(-\tfrac{1}{2}W_2) - \exp(-\tfrac{1}{2}W_1)], \quad |2U_{20}| < W_2 < W_1, \quad (19)$$

$$\left|\frac{dW}{dx/L_{De}}\right| = [\sqrt{2(W-1)}], \quad W < |2U_{20}|, \quad (20)$$

$$\left|\frac{dW}{dx/L_{De}}\right| = \sqrt{2}\,[\exp(W - 2U_{20}) + W - 1], \quad |2U_{20}| < W, \quad (21)$$

$$|\rho_{net}/\rho_0| \simeq 1, \quad W < |2U_{20}|, \quad (22)$$

$$|\rho_{net}/\rho_0| = \exp(W - 2U_{20}) + 1, \quad |2U_{20}| < W. \quad (23)$$

For minority-carrier density elevation we have (Fig. 4)

$$|\Delta N/\Delta N_0|_{W=W_1} - |\Delta N/\Delta N_0|_{W=W_2} = \frac{1}{\sqrt{2}}\int_{W_2}^{W_1}\frac{e^W - 1}{\sqrt{W-1}}dW, \quad W < |2U_{20}|, \quad (24)$$

$$= \sqrt{2}e^{U_{20}}[\exp(\tfrac{1}{2}W_1) - \exp(\tfrac{1}{2}W_2)], \quad |2U_{20}| < W_2 < W_1. \quad (25)$$

For majority-carrier density depression we have (Fig. 5)

$$|\Delta N/\Delta N_0|_{W=W_1} - |\Delta N/\Delta N_0|_{W=W_2} = (\sqrt{2})[(\sqrt{W_1 - 1}) - \sqrt{(W_2 - 1)}], \quad W < |2U_{20}|, \quad (26)$$

$$= \sqrt{2}e^{U_{20}}[\exp(-\tfrac{1}{2}W_2) - \exp(-\tfrac{1}{2}W_1)], \quad |2U_{20}| < W_2 < W_1. \quad (27)$$

This limiting behavior is evident from the various curves and can be used to extrapolate for large values of W beyond the limits presented here.

DETERMINATION OF SURFACE POTENTIAL

In order to solve a specific problem, we have to supply the value of bulk potential (U_{20}) and the surface potential. In the case of semiconductor step junctions, the surface potential is supplied in the form of junction potential once the doping on the two sides is specified.[1] However, for the surface problem, the determination is not straightforward and depends upon the conditions on the other side; i.e., just to name a few, the voltage on the metal plate for the MIS case, the metal work function for a Schottky junction or other pertinent details for a heterojunction. Whatever be the method used to determine W_S (the details are beyond the scope of this paper), once it is known, the procedure from then on is straightforward.

ALGORTHIM FOR USING THE GENERAL SOLUTION

(i) Determine U_{20}; (ii) determine W_S; (iii) determine if it is a case of "depletion" or of "accumulation"; (iv) for accumulation, follow the accumulation curve for each variable (i.e., for each figure); (v) for depletion, follow the depletion curve for the pertinent value of $|U_{20}|$ for each variable.

SOLUTION FOR A TYPICAL PROBLEM

Consider a p-type uniformly doped semi-infinite semiconductor sample with the following parameter values:

$$U_{20} = -10$$

(this corresponds to a doping of $2.2 \times 10^{14}/\text{cm}^3$ for $n_i \simeq 10^{10}/\text{cm}^3$).

$$U_S = +10$$

(this corresponds to the onset of strong inversion). Then $|W_S| = |U_{20} - U_S| = |-10 - 10| = 20$.

Since it is a case of majority-carrier density depression, it is a depletion set problem. Hence, we pick the curve corresponding to $|U_{20}| = 10$ in the depletion set. The surface is positioned at $W_S = 20$. From then on the values of all the relevant variables can be read off from the five figures. The electric field will be pointing from the surface into the bulk.

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The net charge density will be a negative quantity. These are obvious from the physical situation.

CONCLUSION

We have hereby presented a unified solution in terms of the potential, electric field, charge density, and change in mobile-carrier concentrations throughout a uniformly-doped semi-infinite semiconductor sample at equilibrium. This solution can be directly applied to step junctions (i.e., symmetric and asymmetric *pn* and high low), MIS structures, Schottky barrier junctions, and heterojunctions under equilibrium conditions. An analytical approximation to this unified solution will be presented elsewhere.

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