Paul M. Marcus

Calculation of the Capacitance of a Semiconductor Surface, with Application to Silicon

Abstract: The electrostatic problem of finding the surface capacitance of a plane semiconductor surface as a function of applied voltage is formulated and solved. The solution takes account of the space charge distribution in the semiconductor, of a surface dielectric layer, of the possible presence of surface states, and of the exact Fermi-Dirac statistics for the charge carriers. The macroscopic electrostatic problem and microscopic electronic description are kept separate, convenient reduced units are introduced, and the differential capacitance characteristic is expressed in a simple parametric form. For bands of normal form, and for a single-level acceptor or donor surface state, the reduced characteristic depends on eight reduced quantities for general statistics, and on six for the simpler Boltzmann limit; the latter include three quantities describing the surface state level, one for the dielectric layer, one bulk semiconductor parameter, and one contact potential constant which shifts the voltage scale. Explicit calculations are made for silicon at 293°K for various doping levels, dielectric layers, and single-level surface states; the variation of the characteristic dip in the capacitance is exhibited as a function of these parameters.

1. Introduction

The present work obtains the static capacitance of a plane semiconductor surface and dielectric layer, Fig. 1, as a function of applied voltage, and presents a series of these static capacitance characteristics for silicon as an aid in interpretation of capacitance measurements on silicon. The calculation takes due account of the special variation of the space charge in the semiconductor as the potential varies, which has been studied in numerous previous papers[1–4] and which leads to the well-known decrease in the capacitance when the majority carrier concentration diminishes[5–8]. Such capacitance characteristics have been of direct interest in the device called the surface varactor[7,8]; an example of their use in the interpretation of the structure of thin films of silicon dioxide on silicon is given in a recent paper by D. P. Seraphim et al.[1]

This paper extends the practical side of surface capacitance calculations by exhibiting the shape of capacitance characteristics for Si, as the doping level is systematically varied, and showing the effects of sharp surface states of various kinds, strengths, and positions on these shapes.

The theoretical side of surface capacitance calculations is somewhat extended and simplified here by the following features of the discussion, which is self-contained: (1) The macroscopic electrostatic problem is kept separate from the microscopic electronic description so that the problem and its solution can be completely formulated without describing the band structure or mentioning the Fermi level. (2) A systematic simplification is achieved by the immediate introduction of convenient reduced (dimensionless) variables and working with them throughout; this permits easy count of the number of independent parameters which specify a complete reduced characteristic, and contributes to their classification as bulk or intrinsic, semiconductor, dielectric, or metal electrode parameters, etc. (3) A discussion is given of the contact potential constant which appears as an additive constant in the voltage scale, and it is shown to depend on the work function of both the metal electrode and the semiconductor and on the free-surface value of the relative surface potential. (4) The general Fermi-Dirac statistics are re-

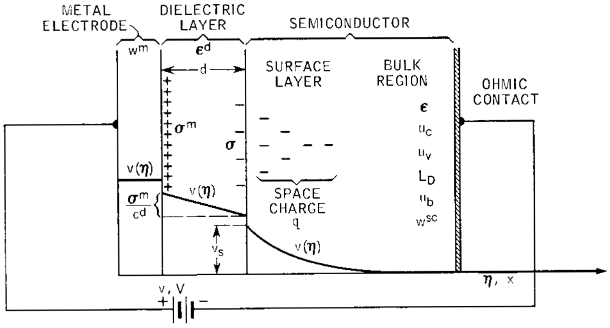

Figure 1 **Configuration for capacitance calculation showing metal electrode, dielectric layer, and semiconductor slab, with external circuit connections.** *The surface charges σ^m and σ and space charge q are indicated, as well as the division of the semiconductor into a surface region and a bulk region, the drop in potential across the dielectric σ^m/c^d and across the surface layer v_s, and the characteristic parameters for each material.*

tained throughout the formulation. Although general statistics are not required to discuss silicon at 293°K, the formulation is then available for application to cases which require it. The formulation is not much more complicated than for Boltzmann statistics; it requires only a simple generalization of the space charge functions of the Boltzmann case.[9]

Section 2 gives the basic definition of the reduced capacitance c and other quantities, and then deduces a simple parametric representation of c and the reduced applied voltage v as functions of the relative surface potential of the semiconductor v_s (relative to bulk material). The discussion here is simple macroscopic electrostatics, hence no mention of the band structure is needed or made. However, the complications of the relation between space charge and potential in the semiconductor, which bring in the electron statistics, are deferred to Section 3, and merely summarized in the total space charge function $F(v_s)$. Explicit discussion of the contact potential difference, which enters the relation between v and v_s, is given within the macroscopic framework. Formal account is taken of the possible presence of a surface charge in surface states on the semiconductor by means of a reduced surface charge density function $\sigma(v_s)$.

Section 3 gives the explicit formula for $F(v_s)$ using the general Fermi-Dirac statistics for the electron distribution; the macroscopic and microscopic problems are related by the usual (Fermi-Thomas) assumption that the electron distribution at a point depends on the local point value of the electrostatic potential in the same way that it would in a constant potential. The simplification that occurs in the low-density approximation when the Fermi-Dirac functions are replaced by exponentials is then given. The results for general statistics depend on just two additional dimensionless intrinsic parameters of the semiconductor (for a conduction and valence band of normal shape).

Section 4 gives explicit formulas for $\sigma(v_s)$ for the two simplest surface state distributions, namely a single acceptor or a single donor level. Three parameters characterize either of these distributions, namely the strength, position, and degeneracy factor of the surface states. These very simple concentrated distributions give the sharpest effects on the problem, i.e., the most abrupt changes in the $c(v)$ curve. In the absence of more specific knowledge, they are used to obtain possible extreme forms of the $c(v)$ curves.

Section 5 specializes the discussion to silicon, gives typical values of the eight parameters entering directly into the $c(v)$ relation and, in Figs. 2 through 9, exhibits the behavior of $c(v)$ as certain of these parameters are systematically varied, particularly the bulk carrier concentration. Table 1 presents corresponding values of the five equivalent parameters that describe the bulk carrier concentration (at 293°K); Table 2 presents various quantities characterizing the minimum in the potential as the bulk carrier concentration varies from strongly n-type to strongly p-type, and Fig. 10 plots the minimum capacitances. The effects of a single-level acceptor or donor surface state of various strengths at various energy levels on $c(v)$ are shown in Figs. 4, 8, and 11.

2. Parametric formula for the capacitance characteristic

The reduced differential capacitance per unit area, c, of a thick plane semiconducting slab in contact with a plane metal electrode through a dielectric layer is defined by

$$c \equiv \frac{1}{(\epsilon/\gamma L_D)} \frac{d\Sigma^m}{dV} \equiv \frac{d\sigma^m}{dv}, \tag{1}$$

where:

Σ^m = charge per unit area on the metal electrode (coulombs/meter^2);

V = applied voltage (volts) = potential of the electrode with respect to the interior (bulk region) of the semiconductor. (The bulk region is far enough from the surface to be beyond the space charge region, hence is uncharged);

ϵ = dielectric constant of the semiconductor (dimensionless);

γ = dimensional constant in Poisson's equation,

$$\frac{\partial^2\phi}{\partial x^2} = -\frac{\gamma\rho}{\epsilon}, \tag{2}$$

in which ϕ = electrostatic potential (volts), ρ = space charge density (coul/meter^3), and $\gamma = 1.131 \times 10^{11}$ volt meter/coul in Gaussian MKSA units.

L_D = the intrinsic Debye length of the semiconductor (meters), defined by

$$L_D \equiv \left(\frac{\epsilon k T}{2e^2 n_i \gamma}\right)^{1/2}, \tag{3}$$

in which kT = absolute temperature in energy units = 4.0446×10^{-21}(T°K/293) joules, e = the electronic charge (1.6021×10^{-19} couls), and n_i = a suitable reference number density of electrons, which will later be defined definitely (see (22)), but will essentially be the intrinsic number density of electrons (or holes) in the semiconductor.

$$\sigma^m = \frac{\Sigma^m}{2n_i e L_D}, \tag{4}$$

which is the reduced charge per unit area on metal electrode (dimensionless) where $2n_i e L_D$(coul/meter^2) has been used as the unit of surface charge density.

$$v = \frac{eV}{kT}, \tag{5}$$

which is the reduced applied voltage (dimensionless).

The general relation between c and v may be expressed implicitly by giving each in terms of the surface potential of the semiconductor, in the form

$$v = v_s + \frac{F - \sigma}{c^d} + w, \tag{6}$$

and

$$\frac{1}{c} = \frac{1}{c^d} + \frac{1}{F' - \sigma'}, \tag{7}$$

where v_s = reduced surface potential of the semiconductor with respect to the bulk ($= e(\phi_{(\text{surface})} - \phi_{(\text{bulk})})/kT$). $F(v_s) = -q$ where q = the total reduced space charge in the semiconductor per unit area of surface = $\int_0^\infty \rho(x)dx/(2n_i e L_D)$ (explicit expressions for F for general Fermi statistics and for Boltzmann statistics will be given in Section 3 in terms of various intrinsic and bulk parameters); $\sigma(v_s)$ = reduced charge per unit area in surface states on the semiconductor surface (explicit expressions for acceptor or donor states at a single level will be given in Section 4); and

$$c^d \equiv \frac{\epsilon^d L_D}{\epsilon d} \tag{8}$$

is the reduced capacitance per unit area of the dielectric layer, $(\epsilon^d/\gamma d)/(\epsilon/\gamma L_D)$, where ϵ^d is the dielectric constant and d is the thickness of the dielectric layer.

The charge per unit area on the metal electrode, which balances the space charge and surface charge on the semiconductor, is therefore

$$\sigma^m = F - \sigma. \tag{9}$$

The total potential rise v in going from the bulk region of the semiconductor to the bulk region (i.e., the interior) of the metal, which is given in Eq. (6), is thus made up of a rise v_s to the surface of the semiconductor, a rise $(F - \sigma)/c^d$ across the dielectric layer, and a part w that is independent of the applied voltage. See Fig. 1. This constant part w, which is essentially a contact potential difference, may be evaluated by considering the behavior of the potential when the metal electrode and semiconductor are in their isolated neutral states, i.e., their free-surface states in which each is separately neutral and no charge has yet been allowed to flow from one to the other to bring their mobile charge distributions into statistical equilibrium, with equalization of the electrochemical potentials. In this isolated neutral state v equals the (reduced) work per unit charge carried from the semiconductor interior to the metal interior, which equals the work per unit charge from semiconductor interior to exterior minus the work per unit charge from metal interior to metal exterior, or

$$v = -w^{sc} + w^m, \tag{10}$$

where

$$w^{sc} = e\chi^{sc}/kT, \; w^m = e\chi^m/kT, \tag{11}$$

χ^{sc} = the work function of the semiconductor = work in carrying unit negative charge from interior to exterior, and χ^m is the similar quantity for the metal. Note that the exteriors of both metal and semiconductor are at the same potential everywhere because the systems are neutral; hence no work is done in carrying a charge between the metal and semiconductor. The neutrality of the free surface state of the semiconductor gives

$$F(v_s^f) = \sigma(v_s^f), \tag{12}$$

where v_s^f is the free-surface value of the relative surface potential. Hence from Eqs. (6), (10), and (12),

$$w = w^m - w^{sc} - v_s^f. \tag{13}$$

If we were dealing with two metals in contact, the constant w would be merely the difference of work functions, and the term v_s^f in Eq. (13) would be missing. The semiconductor case is different, however, in that part of the contact potential difference is taken up over the space charge layer, as well as between surface charges.

Corresponding to the two variable parts which contribute to v in Eq. (6), namely, v_s and $(F - \sigma)/c^d$, the capacitance c in Eq. (7) is made up of two parts, namely,

c^d, and $F' - \sigma' \equiv dF/dv_s - d\sigma/dv_s$. These are (differential) capacitances in series, in each of which the charge per unit area on the metal electrode ($F - \sigma$) is associated with a characteristic potential difference. Thus $F' - \sigma'$ corresponds to the potential change v_s between the bulk and the surface of the semiconductor, and hence is a capacitance referring only to the semiconductor (later called c^{sc}); c^d corresponds to the potential change across the dielectric layer and is the familiar dielectric capacitance given in Eq. (8).[10]

3. Space charge and potential in the semiconductor

Evaluation of $c(v)$ from Eq. (6) and Eq. (7) requires the function $F(v_s)$ relating total space charge (per unit area of surface) in the semiconductor to the relative surface potential v_s. Poisson's equation, Eq. (2), for the potential must be solved with boundary conditions at the surface and in the bulk material. In reduced units the equation and boundary conditions are

$$\frac{d^2v(\eta)}{d\eta^2} = -\bar{\rho}(\eta), \quad v(0) = v_s, \quad v(\infty) = 0, \tag{14}$$

where the reduced distance η, potential $v(\eta)$, and charge density $\bar{\rho}$ are defined by

$$\eta \equiv \frac{x}{L_D}, \tag{15}$$

$$v(\eta) \equiv \frac{e\phi(x)}{kT}, \tag{16}$$

$$\bar{\rho} \equiv \frac{\rho}{2n_i e}. \tag{17}$$

The formulation of the mathematical problem in Eq. (14) is completed by expressing $\rho(\eta)$ in terms of $v(\eta)$ using statistical formulas for the electron distribution. This will be done in the spirit of the Fermi-Thomas approximation using the local value of the potential in formulas for the electron density that hold in a constant potential; this approximation should be rather good here where the potential does not vary appreciably on an atomic scale.

The electrons are assumed to be distributed over conduction and valence bands of normal form according to the Fermi-Dirac distribution law (the simpler approximate formulas for the Boltzmann distribution are given at the end of this section). Then the bulk number densities of electrons n_b and holes p_b can be written[11] in terms of (reduced) chemical potentials for electrons u_n and holes u_p using Fermi-Dirac functions of order one half $\mathcal{F}_{\frac{1}{2}}$. Thus we have

$$n_b = N_c\mathcal{F}_{1/2}(u_n), \tag{18}$$

$$p_b = N_v\mathcal{F}_{1/2}(u_p), \tag{19}$$

where

$$u_n + u_p = -\frac{\epsilon_G}{kT} = -\bar{\epsilon}_G, \tag{20}$$

$$\mathcal{F}_j(x) \equiv \frac{1}{j!}\int_0^\infty \frac{t^j\,dt}{e^{t-x}+1},$$
$$\mathcal{F}_j(x) \xrightarrow[x\to-\infty]{} e^x, \quad \mathcal{F}_j'(x) = \mathcal{F}_{j-1}(x). \tag{21}$$

Thus the bulk behavior is specified by three independent intrinsic parameters which characterize the band structure (N_c, N_v, ϵ_G) and one independent bulk parameter which depends on impurity content and may be any one of n_b, p_b, u_n, or u_p. Further, in introducing dimensionless parameters to replace N_c, N_v, and n_b, it is convenient to define a fifth parameter u_b, which also characterizes the impurity content or doping level. The relations among these five equivalent parameters are tabulated for silicon in Table 1 (page 501). Thus we define intrinsic parameters n_i, u_c, and u_v by

$$n_i^2 \equiv N_c N_v e^{-\bar{\epsilon}_G}, \tag{22}$$

$$e^{-u_c} \equiv N_c/n_i, \tag{23}$$

$$e^{u_v} \equiv N_v/n_i. \tag{24}$$

Then, from Eqs. (23), (24) and (22), followed by (20),

$$u_c - u_v = -\bar{\epsilon}_G = u_n + u_p, \tag{25}$$

hence a bulk parameter u_b can be defined by

$$u_b \equiv u_n - u_c = -u_p - u_v. \tag{26}$$

In the same electron system, which is all in statistical equilibrium, we consider the electron densities at a point where the local (reduced) electrostatic potential is $v(\eta)$. The chemical potential of the electrons is increased there by $v(\eta)$ (in contrast to the electrochemical potential or total chemical potential which is the same everywhere) and that of the holes is decreased by $v(\eta)$. Consequently, using Eqs. (18), (19), (23), (24) and (26), the densities are

$$\begin{aligned} n(\eta) &= n_i e^{-u_c}\mathcal{F}_{1/2}(u_b + u_c + v(\eta)) \\ &\equiv n_i e^{-u_c}\mathcal{F}_{1/2}(u(\eta) + u_c), \end{aligned} \tag{27}$$

$$\begin{aligned} p(\eta) &= n_i e^{u_v}\mathcal{F}_{1/2}(-u_b - u_v - v(\eta)) \\ &\equiv n_i e^{u_v}\mathcal{F}_{1/2}(-u(\eta) - u_v), \end{aligned} \tag{28}$$

where a new measure of the potential has been introduced,

$$u(\eta) \equiv u_b + v(\eta), \tag{29}$$

and we see that u_b is the bulk value of u, while the surface value of u is

$$u_s = u_b + v_s. \tag{30}$$

The reduced space charge density can now be written, assuming the bulk is neutral (on including the contributions of all charged impurity centers), and using Eqs. (27) and (28),

$$\bar{\rho}(\eta) \equiv \frac{\rho(\eta)}{2n_i e} = \frac{p - p_b - (n - n_b)}{2n_i}$$
$$= -\tfrac{1}{2}[f'(u, u_c, u_v) - f'(u_b, u_c, u_v)] \tag{31}$$

where

$$f'(u, u_c, u_v) \equiv e^{-u_c}\mathfrak{F}_{1/2}(u + u_c)$$
$$- e^{u_v}\mathfrak{F}_{1/2}(-u - u_v). \tag{32}$$

Finally Eq. (14) is integrated, using Eq. (31) for $\bar{\rho}$, to give

$$F(v_s) = -q(v_s) = -\int_0^\infty \bar{\rho}\, d\eta = -\frac{dv_s}{d\eta}$$
$$= \operatorname{sign}(u_s - u_b)[f(u_s, u_c, u_v) - f(u_b, u_c, u_v)$$
$$- (u_s - u_b)f'(u_b, u_c, u_v)]^{1/2}, \tag{33}$$

where

$$f(u, u_c, u_v) = e^{-u_c}\mathfrak{F}_{3/2}(u + u_c) + e^{u_v}\mathfrak{F}_{3/2}(-u - u_v), \tag{34}$$

and

$$f'(u, u_c, u_v) \equiv \frac{\partial f}{\partial u} \tag{35}$$

is given in Eq. (32).

Thus Eq. (33) gives the required function, $F(v_s)$; then the function $F'(v_s)$, which appears in Eq. (7), is given by

$$F'(v_s) = [f'(u_s, u_c, u_v) - f'(u_b, u_c, u_v)]/2F(v_s). \tag{36}$$

In the low-density approximation, the arguments of the $\mathfrak{F}_j(x)$ functions are always sufficiently negative for the functions to be accurately represented by exponentials (better than 1% for $x < -4$). Then the parameters u_c, u_v drop out and we have from Eqs. (32), (33), (34) and (36)[12]

$$f(u, u_c, u_v) \cong 2 \cosh u, \tag{37}$$

$$f'(u, u_c, u_v) \cong 2 \sinh u, \tag{38}$$

$$F(v_s) \cong \operatorname{sign}(u_s - u_b)2^{1/2}[\cosh u_s - \cosh u_b$$
$$- (u_s - u_b) \sinh u_b]^{1/2}, \tag{39}$$

and

$$F'(v_s) \cong (\sinh u_s - \sinh u_b)/F(v_s). \tag{40}$$

Also, from Eqs. (18), (19), and (26)

$$n_b \cong n_i e^{u_b} \tag{41}$$

$$p_b \cong n_i e^{-u_b} \tag{42}$$

$$n_b + p_b \cong 2n_i \cosh u_b \tag{43}$$

$$n_b p_b \cong n_i^2 \tag{44}$$

$$\bar{\rho} \cong \sinh u - \sinh u_b. \tag{45}$$

From Eq. (44) we see that n_i may be interpreted in the low-density limit as the intrinsic electron (or hole) density, since intrinsic conditions mean $n_b = p_b$; from Eqs. (41) and (42), $u_b \cong 0$ in intrinsic conditions, and u_b gives directly the increase of actual electron density over intrinsic density.

4. Surface state distributions

The simplest and sharpest surface state distributions consist of a single acceptor level or a single donor level with a certain area density at the surface. The reduced surface charge density σ corresponding to these can be specified by three parameters.

For the acceptor case, an occupied level means a negative charge, hence

$$\sigma(v_s) = \sigma(u_s - u_b) = \frac{-\sigma_a}{1 + \beta_a e^{\bar{\epsilon}_{ac} - u_c - u_s}}, \tag{46}$$

where

$\sigma_a = N_a/2n_i L_D$, N_a = number of acceptors per unit area of surface; (47)

$\bar{\epsilon}_{ac}$ = the reduced energy level of the acceptor with respect to the conduction band edge ϵ_c(i.e., the level is at $\epsilon_c + \epsilon_{ac}$, $\bar{\epsilon}_{ac} = \epsilon_{ac}/kT$); (48)

β_a = the degeneracy factor of the acceptor state, with $\beta_a = \frac{1}{2}$ if the (ionized) acceptor has two states with the same energy, either of which, but not both together, can be filled by an electron; (49)

u_c and u_s are as defined in Eqs. (23) and (30).

Similarly, in the donor case, an unoccupied level means a positive charge, hence

$$\sigma(v_s) = \sigma(u_s - u_b) = \sigma_d\left[1 - \frac{1}{1 + \beta_d e^{\bar{\epsilon}_{dc} - u_c - u_s}}\right]$$
$$= \frac{\sigma_d}{1 + \beta_d^{-1} e^{u_s + u_c - \epsilon_{dc}}}$$
$$= \frac{\sigma_d}{1 + \beta_d^{-1} e^{u_s + u_v - (\bar{\epsilon}_{dc} + \bar{\epsilon}_G)}}, \tag{50}$$

where

$$\sigma_d = N_d/2n_i L_D \tag{51}$$

and N_d is the donor area density;

$\bar{\epsilon}_{dc}$ = the reduced energy level of the donor with respect to the conduction band edge ($\bar{\epsilon}_{dc} + \bar{\epsilon}_G$ is then the position with respect to the valence band edge); and

β_d = the degeneracy factor of the donor state, with $\beta_d = 1/2$ if the (neutral) donor has two states at the same energy, either of which, but not both together, can hold an electron.

Table 1 **Equivalent parameters for the bulk carrier density in silicon at 293°K.**[a]

$n_b(m^{-3})$	$p_b(m^{-3})$	u_b	$\ln(n_b/n_i)$	u_n	u_p
10^{25}	1.41×10^{6}	21.76	21.64	−0.87	−43.50
10^{24}	1.58×10^{7}	19.34	19.33	−3.29	−41.08
10^{23}	1.60×10^{8}	17.03	17.03	−5.60	−38.77
10^{22}	1.60×10^{9}	14.73	14.73	−7.90	−36.47
10^{21}	1.60×10^{10}	12.43	12.43	−10.20	−34.17
10^{20}	1.60×10^{11}	10.12	10.12	−12.51	−31.86
1.60×10^{11}	10^{20}	−10.12	−10.12	−32.75	−11.61
1.60×10^{10}	10^{21}	−12.43	−12.43	−35.06	−9.30
1.60×10^{9}	10^{22}	−14.73	−14.73	−37.36	−7.00
1.60×10^{8}	10^{23}	−17.03	−17.03	−39.66	−4.70
1.55×10^{7}	10^{24}	−19.38	−19.37	−42.01	−2.36
1.17×10^{6}	10^{25}	−21.95	−21.96	−44.59	−1.22

[a] Relations among the quantities above are given by: $n_b = 2.718 \times 10^{25}\, \mathfrak{F}_{\frac{1}{2}}(u_n) \cong n_i e^{u_b}$, $p_b = 1.098 \times 10^{25}\, \mathfrak{F}_{\frac{1}{2}}(u_p) \cong n_i e^{-u_b}$, $n_i = 4.012 \times 10^{15}\, m^{-3}$, $u_n + u_p = -44.37$, and $u_b = u_n + 22.63 = -u_p - 21.73$. See Equations (18), (19), (41), (42), (20), (26), (22), (23), and (24).

The function σ' in Eq. (7) has the form, from Eqs. (46) and (50),

$$\sigma'(v_s) \equiv \frac{d\sigma}{dv_s} = \sigma\left(1 + \frac{\sigma}{\sigma_a}\right) \quad \text{(acceptor case)}, \tag{52}$$

$$\sigma'(v_s) = -\sigma\left(1 - \frac{\sigma}{\sigma_d}\right) \quad \text{(donor case)}. \tag{53}$$

5. Parameter values and capacitance characteristics for silicon

• *Parameter dependences*

The parametric equations, Eqs. (6) and (7), for the reduced characteristic $c(v)$ depend on eight reduced quantities for general (Fermi-Dirac) statistics and on six for Boltzmann statistics. (We assume bands of normal form and a single-level acceptor or donor state).

For the semiconductor in the general case three parameters enter into $F(v_s)$, as shown by Eq. (33). These are the intrinsic quantities u_c and u_v and the bulk quantity u_b; however, for Boltzmann statistics, Eq. (39) shows that u_c and u_v drop out.

The dielectric layer enters only through the reduced capacitance c^d given in Eq. (8).

The single-level acceptor or donor function $\sigma(v_s)$ depends on three parameters: σ_a, $\bar{\epsilon}_{ac}$, β_a or on σ_d, $\bar{\epsilon}_{dc}$, β_d, as shown by Eqs. (46) and (50).

Finally, the contact potential constant w in Eq. (6), which translates the voltage scale, is expressed in terms of the work functions of the semiconductor and the metal electrode, Eq. (13), and of v_f^e, the free-surface value of v_s, determined by Eq. (12).

• *Intrinsic parameters and reduced unit sizes for silicon*

The values of u_c and u_v are given by Eqs. (22), (23), and (24) in terms of N_c, N_v, and $\bar{\epsilon}_G$. For calculation at 293°K ($kT = 4.0446 \times 10^{-21}$ joules), we take $\epsilon_G = 1.12\text{eV} = 1.794 \times 10^{-19}$ joules, $N_c = 2.718 \times 10^{25} m^{-3}$, and $N_v = 1.098 \times 10^{25} m^{-3}$. Then $\bar{\epsilon}_G = 44.37$, $n_i = 4.012 \times 10^{15} m^{-3}$, $u_c = -22.63$, and $u_v = 21.73$.

From these intrinsic parameters, the magnitudes of the units used in defining reduced quantities may be calculated as: unit of length $L_D = 4.564 \times 10^{-5} m$, based on Eq. (3) with $\epsilon = 12$, $e = 1.6021 \times 10^{-19}$ couls, and n_i and kT as given above; unit of charge density $2n_ie = 1.2855 \times 10^{-3}$ couls/m^3; unit of surface charge density $= 2n_ieL_D = 5.867 \times 10^{-8}$ coul/m^2; unit of surface density $= 2n_iL_D = 3.662 \times 10^{11} m^{-2}$; unit of capacitance per unit area $= (\epsilon/\gamma L_D) = 2.325 \times 10^{-6}$ farads/m^2; and unit of potential $= (kT/e) = (0.02525)$ volts (1 volt = 39.61 units).

• *Capacitance characteristic curves for silicon with no surface charge*

The effect of systematic variation of bulk carrier concentration on $c(v)$ curves for Si is shown in Figs. 2 through 10. The parameter u_b varies in steps of 5 from +20 (strongly n-type) to −15 (moderately p-type); corresponding values of other measures of bulk carrier concentration are presented in Table 1. Note that the range $|u_b| = 15$ to 20 covers the range n_b or $p_b = 10^{16}/\text{cm}^3$ to $2 \times 10^{18}/\text{cm}^3$, the usual range of physical interest. Only for $|u_b| \geq 20$, i.e., large carrier concentration, does the exact value of u_b (in column 3) for a given majority carrier concentration, differ significantly from the Boltzmann approximation $\ln(n_b/n_i)$ (in column 4). Also for these large carrier concentrations (majority carrier greater than 10^{18} cm^{-3}) the product n_bp_b is less than n_i^2, and the values of $|u_b|$ and of the minority carrier concentrations are unsymmetrical for the same majority carrier concentration—whereas both these relations hold in the Boltzmann region. Since Table 1 shows that in the range of physical interest the Boltzmann approximation holds well, it has been used in all the calculations given here.

The results given in Figs. 2 through 9 also all assume $c^d = 36.63$, corresponding to a dielectric layer with $\epsilon^d = 3.85$ and $d = 4 \times 10^{-7}$m, and all but the dashed curves of Figs. 4 and 8 assume that the surface state density is zero. In the absence of specific knowledge, w has been taken as zero; alternatively, the v scale in each figure can be interpreted as a $(v - w)$ scale.

The curves in Figs. 2 to 9 all show that, for sufficiently positive or negative v, c returns to the asymptotic value c^d, corresponding to the semiconductor capacitance $c^{sc} = F' - \sigma'$ becoming large when the carrier density of electrons or holes near the surface becomes large, and the smaller dielectric capacitance dominates. At an intermediate v the carrier density diminishes and c^{sc} and c have a minimum. This occurs when v and v_s oppose u_b, and requires that $|v_s|$ be somewhat greater than $|u_b|$ (values up to a factor of two are shown in Table 2); we note, however, that although $u(\eta)$ then changes sign between the surface and bulk, $v(\eta)$ and $\rho(\eta)$ do not. The dip in c is seen to be shallower for larger $|u_b|$, to become quite asymmetric at large $|u_b|$ with c returning to c^d much more slowly on the majority carrier side; $c(v)$ for a given u_b is symmetric with $c(v)$ for the negative of that u_b.

The values of various quantities at the minimum in c are tabulated in Table 2. For large bulk carrier densities ($|u_b| \sim 20$) remarkably large values of the applied voltage at the minimum v_m are required (90 volts); the dip is then quite smooth and shallow (2%). (See Fig. 2.) Most of this large v appears across the dielectric, while the drop across the semiconductor v_{sm} is quite small ($\sim$1 volt). Also tabulated are c_m and c_m^{sc} (the values of c and c^{sc} at the minimum), d_m^{sc} (the equivalent thickness of semiconductor with capacitance c_m^{sc}), and $4.605/(\cosh u_b)^{1/2}$ (an estimate of the depth containing 99% of the space charge which is calculated as if the asymptotic exponential for $v(\eta)$ and $\rho(\eta)$ held up to the surface). Both these thicknesses become very small fractions of L_D as $|u_b|$ approaches 20. Finally the total space charge at the minimum q_m is tabulated, and becomes quite large for large $|u_b|$, corresponding to the large increase in c_m^{sc}. Note that the values of c_m^{sc}, u_{sm}, and q_m permit calculation of c_m and v_m at any d (for zero surface state density). In Fig. 10, c_m and c_m^{sc} are plotted against u_b, showing how c_m^{sc} breaks away from c_m as c^d is approached; curves for d = 4000 Å, 2000 Å, and 1000 Å are shown.

• *Surface state effects on the characteristics for silicon*

In Figs. 4, 8, and 11 the effects of single-level surface states on the $c(v)$ curve are shown for various types (acceptor or donor), energy levels, and strengths. They are all shown superposed on the $c(v)$ curve for zero surface state density for $u_b = +$ or -10, which shows a well-defined dip with a characteristic shape.

Table 2 **Capacitance, potential, and space charge at the capacitance minimum for silicon at 293°K with zero surface charge.**

u_b	*Majority carrier concentration* cm^{-3}	v_m	v_{sm}	c_m	c_m^{sc}	d_m^{sc}/L_D	$\frac{4.605}{(\cosh u_b)^{\frac{1}{2}}}$	q_m
0	4.01×10^9	0.00	0.00	0.97	1.00	1.00	4.61	0.00
±5	5.95×10^{11}	∓8.43	∓7.57	2.40	2.57	0.39	0.53	$\pm 3.143 \times 10^1$
±7.5	7.25×10^{12}	∓15.86	∓12.0	5.67	6.71	.15	.15	$\pm 1.413 \times 10^2$
±10	8.84×10^{13}	∓32.62	∓16.6	12.68	19.39	.052	.044	$\pm 5.868 \times 10^2$
±11	2.40×10^{14}	∓46.47	∓18.5	16.52	30.10	.033	.027	$\pm 1.025 \times 10^3$
±12	6.53×10^{14}	∓68.95	∓20.4	20.59	47.02	.021	.016	$\pm 1.778 \times 10^3$
±13	1.77×10^{15}	∓106.2	∓22.3	24.48	73.80	.014	.0098	$\pm 3.072 \times 10^3$
±14	4.82×10^{15}	∓168.5	∓24.2	27.86	116.3	.0086	.0059	$\pm 5.285 \times 10^3$
±15	1.31×10^{16}	∓273.5	∓26.1	30.55	184.0	.0054	.0036	$\pm 9.066 \times 10^3$
±16	3.57×10^{16}	∓451.5	∓28.0	32.54	292.0	.0034	.0022	$\pm 1.551 \times 10^4$
±17	9.69×10^{16}	∓752.9	∓30.0	33.95	464.5	.0022	.0013	$\pm 2.648 \times 10^4$
±18	2.63×10^{17}	∓1262	∓31.9	34.90	740.7	.0014	.00080	$\pm 4.506 \times 10^4$
±19	7.16×10^{17}	∓2125	∓33.8	35.53	1184	.00084	.00049	$\pm 7.659 \times 10^4$
±20	1.95×10^{18}	∓3584	∓35.8	35.93	1895	.00053	.00030	$\pm 1.300 \times 10^5$

In the table above: v_m = total potential difference at minimum c; v_{sm} = potential drop between semiconductor surface and bulk at minimum; c_m = total capacitance (per unit area) at minimum; c_m^{sc} = capacitance (per unit area) of semiconductor at minimum $= F' - \sigma'$; $d_m^{sc}/L_D \equiv 1/c_m^{sc}$ = equivalent thickness in Debye lengths of semiconductor with capacitance c_m^{sc}; $4.605/(\cosh u_b)^{\frac{1}{2}}$ = approximate depth (in Debye lengths) containing 99% of space charge, assuming asymptotic form for $v(\eta)$, $p(\eta) \sim \exp[-(\cosh u_b)^{\frac{1}{2}}\eta]$; and q_m = total space charge in semiconductor at minimum $= -F(v_{sm})$.

The tabulated majority carrier concentration $= n_b$ for $u_b > 0$, p_b for $u_b < 0$; it is computed from $4.012 \times 10^9 e^{|u_b|}$ cm^{-3}. For all results in the table it has been assumed that $c^d = 36.63$ ($d = 4 \times 10^{-7}$, $\epsilon = 3.85$), and $\sigma = \sigma' = 0$ (no surface charge).

The total and partial voltages and capacitances above are related by $v_m = v_{sm} - q_m/c^d$, and $1/c_m = 1/c_m^{sc} + 1/c^d$. Values of c_m and v_m at arbitrary dielectric thickness d_1, dielectric constant $\epsilon_1{}^d$ (and the same u_b, and zero surface charge) may then be calculated using $c^{d1} = (4 \times 10^{-7}\epsilon_1{}^d/d_1 3.85)c^d$ for c^d.

Figures 2–9 **Reduced surface capacitance, c(v), for n-type, p-type, or intrinsic silicon at 293°K.** *Applicable conditions, parameters, and materials are indicated within each Figure. In Figs. 4 and 8, dashed lines show the effect on* $c(v)$ *of an acceptor state with the parameters given.*

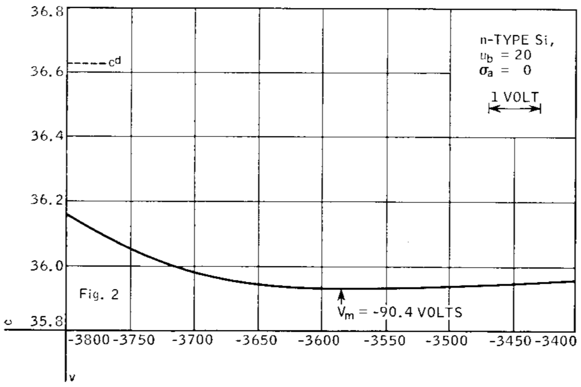
Fig. 2

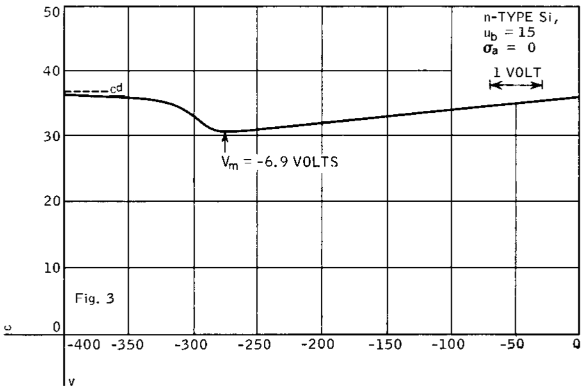
Fig. 3

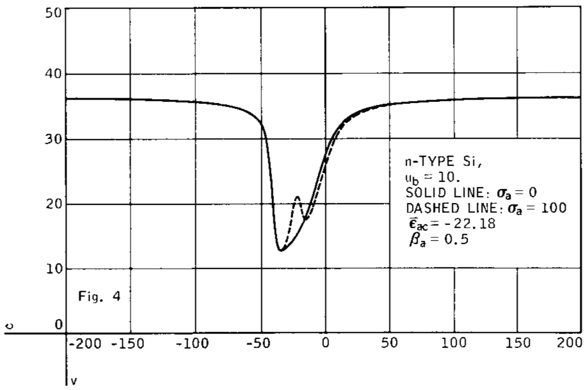
Fig. 4

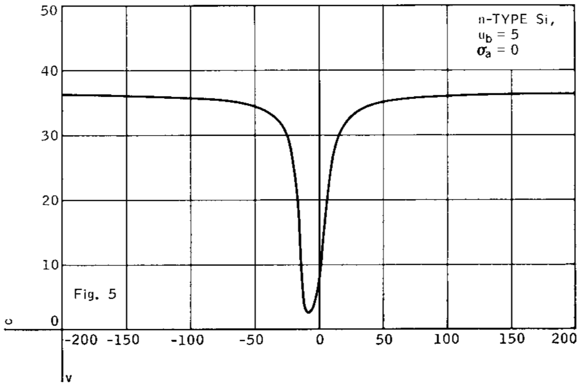
Fig. 5

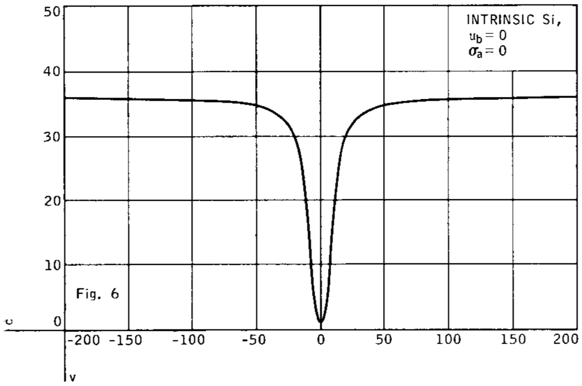
Fig. 6

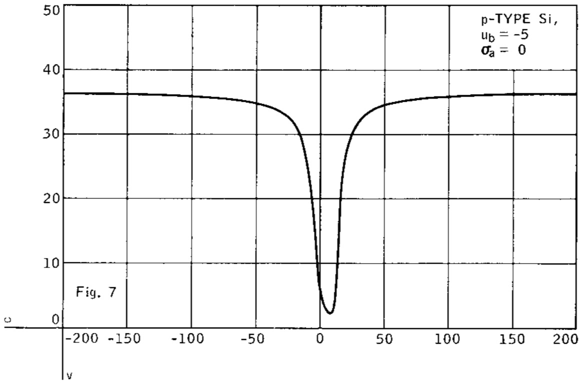
Fig. 7

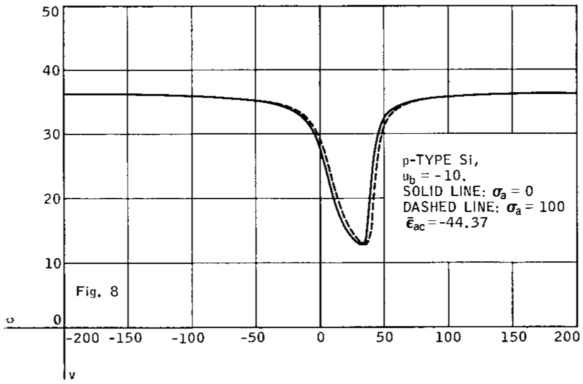
Fig. 8

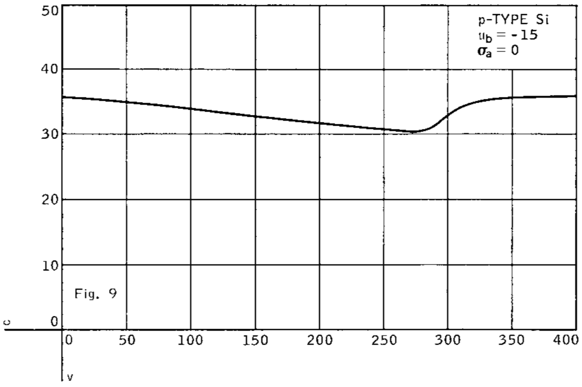
Fig. 9

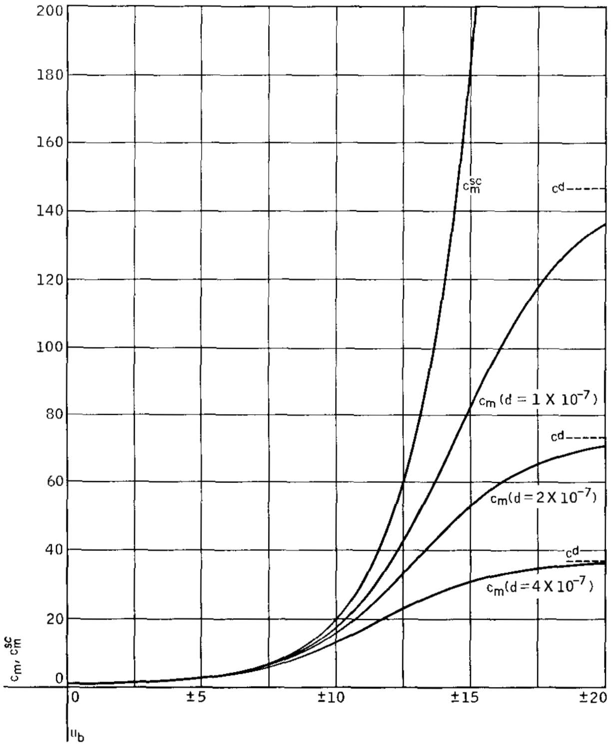

Figure 10 **Reduced surface capacitance of silicon at 293°K at the minimum of the c(v) curve, as a function of the doping level specified by u_b;** *c_m^{sc} is the value for the semiconductor alone; c_m is the value when dielectric layers of various thicknesses d are present. The limiting dielectric capacitance c^d is indicated by broken lines appearing above each curve.*

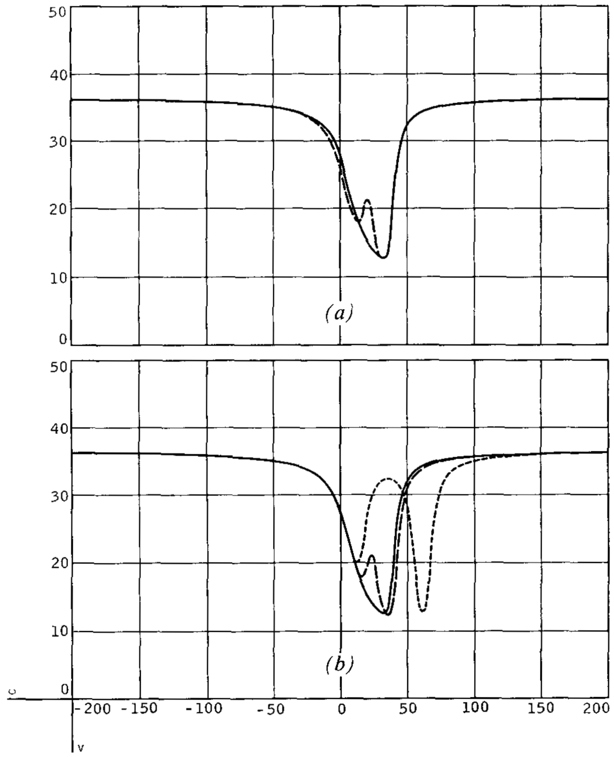

Figure 11 **Reduced surface capacitance characteristic, c(v), for p-type silicon, with $u_b = -10$.** *Figure 11a is for silicon with and without a single-level midgap donor state (the dashed and continuous curves respectively) with $\sigma_d = 100$, $\bar{\epsilon}_{do} = -22.18$, and $\beta_d = 0.5$. Figure 11b is for silicon without a single-level midgap acceptor state (the solid curve) and with acceptor states in two strengths: $\sigma_a = 100$, $\bar{\epsilon}_{ao} = -22.18$, and $\beta_a = -0.5$ (the dashed curve); and $\sigma_a = 1000$, $\bar{\epsilon}_{ac} = -22.18$, and $\beta_a = 0.5$ (the dotted curve.)*

The dashed lines in Figs. 4 and 11a show the similar effects of a midgap acceptor state ($\bar{\epsilon}_{ac} = -22.18$) on n-type material ($u_b = +10$) and a midgap donor state on p-type material ($u_b = -10$); these are symmetrical when, as here, the surface states have the same strength. In the cases shown $\sigma = 100$, corresponding to the moderate surface state density of $3.66 \times 10^9/\text{cm}^2$ (and a free surface potential $v_s^f = -1.1$ for the n-type and $+1.1$ for the p-type material). At applied voltage $v = 0$, the surface state in each case is fully charged, hence the surface state contribution to the capacitance $-\sigma'$ is negligible (see Eq. (7)), but the surface potential is changed in such a direction as to decrease F', the space charge contribution to the capacitance (again, see Eq. (7)), and the $c(v)$ curve falls below the curve for zero surface state density. As v changes toward the value for minimum $c(v)$, (corresponding to driving out the majority carrier), the surface state charge decreases (the acceptor empties, the donor fills) and the capacitance c^{sc} increases, giving rise to a peak. Then as v goes past the minimum to increase the minority carrier concentration, the surface state becomes completely uncharged and c^{sc} returns quickly to the value for zero surface state density.

For a midgap acceptor surface state in p-type material, Fig. 11b shows that the peaked structure in the center of the dip is the same, but now the acceptor is charged on the minority carrier side of the minimum. In contrast to Fig. 11a the $c(v)$ curve now falls below the curve for zero surface state density on that side of the minimum (toward positive v). If the surface state density is increased to $\sigma_a = 1000$ (3.66×10^{10} states/cm^2), Fig. 11b shows that the effects on the side of the dip where the surface states are charged are greatly increased.

Finally we note that if the surface acceptor in p-type material has its energy level at the top of the valence band

($\bar{\epsilon}_{ac} = -44.37$), this is low enough so that the state is filled and charged throughout the voltage range of the dip. Then, as shown in Fig. 8, the surface state merely shifts the voltage scale by σ_a/c^d (see Eq. (6)), but does not contribute to the capacitance; it acts like the dashed line in Fig. 11a on the right side of the dip. However, if the acceptor should be at the bottom of the conduction band ($\bar{\epsilon}_{ac} = 0$), it remains empty and neutral throughout the dip, and the $c(v)$ curve is not significantly changed from the curve for zero surface state density.

Acknowledgments

The author is indebted to Dr. D. R. Young of the IBM Components Division for introducing him to this problem, and to Dr. D. P. Seraphim of the IBM Research Division for his encouragement and interest.

References and footnotes

1. D. P. Seraphim et al., *IBM Journal* **8**, 400 (1964).
2a. R. H. Kingston and S. F. Neustadter, *J. Appl. Phys.* **26**, 718 (1955).
2b. C. G. B. Garrett and W. H. Brattain, *Phys. Rev.* **99**, 376 (1955).
3. R. Seiwatz and M. Green, *J. Appl. Phys.* **29**, 1034 (1958).
4. D. R. Frankl, *J. Appl. Phys.* **31**, 1752 (1960). (A review of the literature of calculations on the space charge region at a semiconductor surface is given.)
5. D. R. Frankl, *Solid State Elect.* **2**, 71 (1961).
6. R. Lindner, *Bell Syst. Tech. J.* **16**, 803 (1962).
7. L. Terman, *Solid State Elect.* **5**, 285 (1962).
8. A. E. Feuersanger and D. R. Frankl, *IEEE Trans. Prof. Group on Electron Devices* **ED-10**, 143 (1963).
9. General statistics are also retained in the work of Seiwatz and Green[3]. The discussion here appears somewhat simpler because of the separation of electrostatic problem and electronic description, the use of reduced units, and the use of parallel notation for the space charge functions in the Fermi-Dirac and Boltzmann cases.
10. More formally, Eq. (7) follows immediately by differentiating Eq. (6) with respect to σ^m, and using Eqs. (1) and (9).
11. See, for example, J. S. Blakemore, *Semiconductor Statistics*, Pergamon Press, 1962, pp. 79, 81. Note that the Fermi-Dirac functions are defined here with the more convenient Dingle normalization, rather than the McDougall-Stoner normalization used in Ref. 3.
12. The function $F(v_s)$ in Eq. (39) is the same function introduced in Ref. 2a, but with a sign added to give a continuous monotonically increasing function; this is the opposite choice of sign to that used in Ref. 4.

Received June 16, 1964.