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Analysis of Field-Aided, Charge-Coupled Device Transfer

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We study the numerical solution of a nonlinear, partial-differential equation that describes charge transport in a model of a charge-coupled device (CCD). This model differs from previous models in that field-aiding of the transfer is taken into account. Although a derivation of the transport equation is given, the main emphasis in the paper is on the numerical techniques involved, and no actual numbers are presented. Actual numerical results based on the techniques developed here can be found in several recent design studies. The equation, which is parabolic, has one space dimension and one time dimension. Galerkin's method, with standard chapeau functions, is used to discretize in space. This results in a very stiff system of nonlinear, ordinary, differential equations. To solve these equations, we use a first-order backward Euler scheme coupled with extrapolation. A number of alternative schemes were tried and found to be inadequate.

I. INTRODUCTION

In this paper, we study the numerical solution of a nonlinear, partial-differential equation that describes charge transport in a model of a charge-coupled device (CCD). The emphasis is on the numerical techniques involved, although a derivation of the equation is given. The reader is referred to other papers where the solutions are used in device theory and design.[1,2] We briefly summarize the physical background of the equation first.

A knowledge of the dynamics of charge transfer in a CCD is, of course, central to a complete understanding of its operation. A calculation of the motion of charge in a CCD, starting from the coupled, nonlinear Poisson and charge-conservation equations and taking into account the full geometry of the device, has so far proved impossible. However, Strain and Schryer[3] and, independently, Kim and Lenzlinger[4] developed and studied an approximate, one-dimensional model of charge transfer in a CCD. The original analysis considered motion owing only to diffusion and the mutual repulsion of the charge carriers. Field-aided transfer was ignored. Since these original studies, a number of other authors have studied the effects of field-aiding.[5–8] In Refs. 5, 6, and 8, as in the original papers,[3,4] an infinite sink for the charge at one end of a cell is assumed. The assumption of an infinite sink rules out charge "bunching," which in certain situations is an important effect (for an example of this, see Ref. 1, Fig. 8). In Ref. 7, the assumption of an infinite sink is not made. In this paper, we extend the original work[3,4] to include field-aiding and more realistic boundary conditions. Our model can describe both surface[9] CCDs and buried-channel[10] CCDs (BCCDs). We do not include the effects of surface traps, since the main application[1] was to BCCDs. We feel the numerical scheme described here has advantages over that used in Ref. 7, where essentially the same model as ours was used to study surface CCDs, with the effect of traps included. Calculations using our methods show that BCCDs, which can be fabricated with present technology, should be extraordinarily fast and efficient and have reasonable charge-carrying capabilities. Transfer times of 1.8 ns are predicted for a two-phase device having 10-μm-wide electrodes.[1] Slower but similar results are obtained for surface devices.

Strain and Schryer[3] solved, by the method of finite differences, a transport equation quite similar to the one we study here. However, their method of solution proved inadequate when applied to our equation. It is possible to obtain solutions of the transport equation as follows. We use Galerkin's method[11] with standard chapeau functions in space. We treat the time behavior by polynomial extrapolation to the limit of the results of a first-order, fully implicit (nonlinear), finite difference scheme. Although the equation only roughly models the true physical situation, an accurate knowledge of the solution as it varies over many orders of magnitude is necessary if it is to be of any use. This requirement makes the numerical solution of the equation difficult. Many other schemes were tried, and the above method is the only one we found that could solve the problem.

The equation of charge transport is derived in Section II, although some more complex details are given in Appendix A. The technique

for numerically solving the equation of charge motion is given in Section III, with some details in Appendix B. Questions of existence and accuracy are discussed in Section IV, along with the use of polynomial extrapolation. An outline of the theory of extrapolation is given in Appendix C. The method by which initial solutions are obtained is the subject of Section V. Finally, in Section VI we discuss several other schemes by which we tried to solve the equation of charge motion and which failed.

II. DERIVATION OF THE TRANSPORT EQUATION

We refer the reader to the literature for a discussion of the principles of operation of either surface CCDs[9] or BCCDs.[10] Basically, however, both are devices that move packets of charge from under one electrode to under another electrode by suitably changing the voltage on the electrodes.

As in Ref. 3, we assume that the charge can be described by a charge density $q(x, t)$. Here, x is the distance under the plates (see Fig. 1) and t is the time. Then, as we show in Appendix A, the component of the electric field along the direction of motion of the charge, which is due to the mutual repulsion of the charge, is

$$E_x^q = -Sq_x. \tag{1}$$

The elastance S is assumed to be a constant independent of x and t. In all that follows, we use subscripts to denote differentiation; thus, $q_x = \partial q(x, t)/\partial x$, etc. Equation (1) holds for both surface and buried

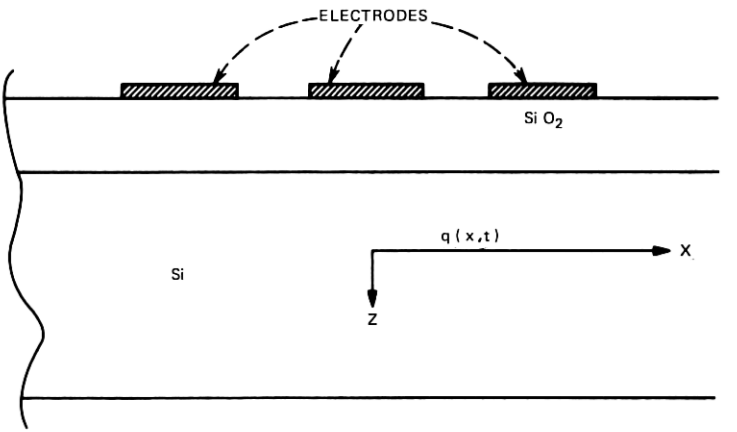

Fig. 1—Schematic of a CCD showing relation to device of x-coordinate in transport equation.

channel devices, although the values of S are different in each case. Expressions for S are given in Appendix A in terms of the physical parameters of the devices.

Let $\varphi(x, t)$ be the given driving potential due to the voltages applied to the electrodes. For a surface CCD, φ is the electric potential at the oxide semiconductor interface, while, for a BCCD, φ is the potential at the potential minimum of the buried channel. In most applications, we have approximated φ by the potential in the CCD in the absence of any mobile charge.[12,13]

The total field along the direction of motion is

$$E_x = -Sq_x - \varphi_x. \tag{2}$$

The current density is[9]

$$J(x, t) = q\mu E_x - Dq_x, \tag{3}$$

where D is the diffusion constant and μ is the mobility, which we also assume to be constant. If we substitute (2) into (3) and make use of the Einstein relation $D = (kT/e)\mu = \alpha\mu$, then

$$J(x, t) = -\mu[(\alpha + Sq)q_x + q\varphi_x]. \tag{4}$$

If we substitute (4) into the charge-conservation equation,[14]

$$q_t + J_x = 0, \tag{5}$$

we get the desired transport equation,

$$q_t = \mu[(\alpha + Sq)q_x + q\varphi_x]_x. \tag{6}$$

The appropriate solution of (6) satisfies an arbitrarily given initial distribution of charge $q(x, 0)$ and the boundary conditions $J(0, t) = J(L, t) = 0$. The boundary conditions state that there is no charge flow into or out of the device at either end. L is the length of the device.

It is convenient to write (6) in terms of dimensionless quantities, as in Ref. 3. Let

$$\tau = t/(L^2/\mu v_0), \quad y = x/L, \quad w = Sq/v_0, \quad \Phi = \varphi/v_0, \quad \beta = \alpha/v_0, \tag{7}$$

where v_0 is a reference voltage. Then (6) becomes

$$w_\tau = [(w + \beta)w_y + w\Phi_y]_y. \tag{8}$$

As it turns out, there seems to be no natural voltage unit in the problem (Ref. 3), so we typically pick $v_0 = 1$ volt.

Physically, the quantity of interest is the total charge present between any two points $0 \leqq y_1 < y_2 \leqq 1$. This suggests that, instead of $w(y, \tau)$, we consider

$$Q(y, \tau) = \int_0^y w(\xi, \tau)d\xi. \tag{9}$$

If we integrate eq. (8) with respect to y from 0 to y and make use of the boundary condition $J(0, t) = 0$, we get

$$Q_\tau = (Q_y + \beta)Q_{yy} + Q_y\Phi_y. \tag{10}$$

Since the right-hand side of (10) is just proportional to $J(y, \tau)$, we see that $Q_\tau(1, \tau) = 0$. From this last remark and (9), it follows that the correct boundary conditions on $Q(y, \tau)$ are

$$Q(0, \tau) = 0, \qquad Q(1, \tau) = Q_T = \text{const.} \tag{11}$$

The appropriate initial condition is determined from $w(y, 0)$ by setting $\tau = 0$ in (9). The transport problem we wish to solve is, thus, eq. (10), subject to boundary conditions (11) and given initial conditions. This is a much simpler problem than attempting to solve (8) for the charge density.

III. SOLUTION OF THE TRANSPORT EQUATION

We simplify the notation slightly by setting

$$\psi(y, \tau) = \Phi_y(y, \tau), \tag{12}$$

and note that (10) can be written

$$-\beta Q_{yy} - \frac{1}{2}\frac{\partial}{\partial y}(Q_y)^2 - \psi Q_y + Q_\tau = 0. \tag{13}$$

If we multiply both sides of (13) by a continuous, piece-wise differentiable function $f(y)$ which satisfies $f(0) = f(1) = 0$, integrate the result from 0 to 1, and integrate the terms containing second derivatives by parts, we obtain (letting $f' = df/dy$)

$$\int_0^1 \{[\beta Q_y + \tfrac{1}{2}(Q_y)^2]f'(y) + [-\psi Q_y + Q_\tau]f(y)\}dy = 0. \tag{14}$$

Equation (14) is the starting point for the application of Galerkin's method, because any twice-differentiable function $Q(y, \tau)$ that satisfies (14) for all continuous, piece-wise differentiable $f(y)$ satisfying $f(0) = f(1) = 0$ must also be a solution of (13).

We now discretize in space by introducing a net $\{y_1, y_2, \cdots, y_N\}$ on $[0, 1]$ and a set of standard chapeau functions $f_j(y)$, $1 \leqq j \leqq N$, as pictured in Fig. 2 and defined in Appendix B. In all that follows, the

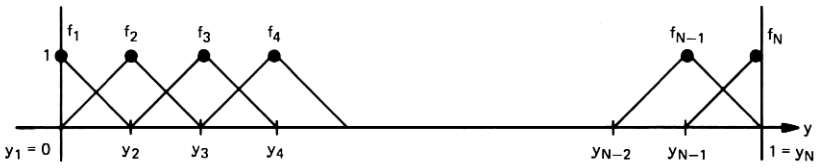

Fig. 2—Discretization of the space interval and the corresponding chapeau functions.

net $\{y_1, \cdots, y_N\}$ is assumed to be given and fixed. In terms of the basic chapeau functions, we define approximations to the solution and external field:

$$\tilde{Q}(y, \tau) = \sum_{j=2}^{N-1} Q_j(\tau) f_j(y) + Q_T f_N(y), \tag{15}$$

$$\tilde{\psi}(y, \tau) = \sum_{j=1}^{N} \psi_j(\tau) f_j(y). \tag{16}$$

Note that $\tilde{Q}(y, \tau)$ has been constructed to satisfy the boundary conditions, $\tilde{Q}(0, \tau) = 0$, $\tilde{Q}(1, \tau) = Q_T$. The functions $Q_j(\tau)$ are yet to be determined, but we require that they satisfy the initial conditions

$$Q_j(0) = Q(y_j, 0). \tag{17}$$

Because of (17), $\tilde{Q}(y, \tau)$ satisfies the correct initial conditions at the mesh points: $\tilde{Q}(y_j, 0) = Q(y_j, 0)$. We define $\psi_j(\tau) = \psi(y_j, \tau)$, so that $\tilde{\psi}(y_j, \tau) = \psi(y_j, \tau)$.

To determine the $N - 2$ functions $Q_j(\tau)$, we require that $\tilde{Q}(y, \tau)$ satisfy (14) for each of the $N - 2$ choices of $f(y)$, $f(y) = f_j(y)$, $2 \leqq j \leqq N - 1$, with $\psi(y, \tau)$ replaced by $\tilde{\psi}(y, \tau)$. This yields a system of $N - 2$ first-order, nonlinear, ordinary differential equations for the $Q_j(\tau)$. This technique has a robust history and has been applied, not only to many problems of the same type as (13), but to other types of problems as well. The idea is quite simple: Let the approximate solution be a linear combination of the functions f_j, $2 \leqq j \leqq N - 1$ and then make the left-hand side of (13) orthogonal to each of these functions. In geometrical terms, this means making the left-hand side of (13) orthogonal to the span of $f_2, \cdots, f_{N-1}$, denoted by $\langle f_2, \cdots, f_{N-1} \rangle$, in $\mathcal{L}^2[0, 1]$ in the usual inner product: $(f, g) = \int_0^1 f(y)g(y)dy$. Then, crudely speaking, as more points y_j are chosen, $\langle f_2, \cdots, f_{N-1} \rangle$ spans more of $\mathcal{L}^2[0, 1]$ and the left-hand side of (13) must go to zero as $N \to \infty$, so long as it remains orthogonal to $\langle f_2, \cdots, f_{N-1} \rangle$.

If we carry out the substitution of (15) and (16) into (14), with $f(y) = f_i(y)$, $2 \leqq i \leqq N - 1$, the $N - 2$ equations result:

$$\begin{aligned} \sum_{j=2}^{N-1} Q_j \left[\beta \int_0^1 f_j' f_i' dy - \sum_{k=1}^{N} \psi_k \int_0^1 f_j' f_k f_i' dy + Q_T \int_0^1 f_j' f_i' f_N' dy \right] \\ + \tfrac{1}{2} \sum_{j,k=2}^{N-1} Q_j Q_k \int_0^1 f_j' f_k' f_i' dy + \sum_{j=2}^{N-1} \dot{Q}_j(\tau) \int_0^1 f_j f_i dy \\ = - \left[\frac{Q_T^2}{2} \int_0^1 f_i' (f_N')^2 dy + Q_T \left(\beta \int_0^1 f_i' f_N' dy \right. \right. \\ \left. \left. - \sum_{k=1}^{N} \psi_k \int_0^1 f_k f_N' f_i dy \right) \right]. \end{aligned} \tag{18}$$

In (18) $\dot{Q}_j(\tau) = dQ_j/d\tau$. The values of the integrals appearing in (18) are listed in Appendix B. If we define $h_i = y_i - y_{i-1}$, $2 \leqq i \leqq N$, and substitute into (18) the values of the integrals, we get

$$\begin{aligned}(h_i\dot{Q}_{i-1} + 2(h_i + h_{i+1})\dot{Q}_i + h_{i+1}\dot{Q}_{i+1})/6 \\ + Q_{i-1}[-\beta/h_i + (\psi_{i-1} + 2\psi_i)/6] + Q_i[\beta(1/h_i + 1/h_{i+1}) \\ + (\psi_{i+1} - \psi_{i-1})/6 + \delta_{i,N-1}Q_T/(h_N)^2] + Q_{i+1}[-\beta/h_{i+1} \\ - (\psi_{i+1} + 2\psi_i)/6] + \tfrac{1}{2}\{(Q_i - Q_{i-1})^2/h_i^2 - (Q_{i+1} - Q_i)^2/h_{i+1}^2\} \\ = \delta_{i,N-1}[Q_T^2/(2h_N^2) + Q_T(\beta/h_N + \psi_{N-1}/3 + \psi_N/6)], \quad (19)\end{aligned}$$

where $\delta_{i,N-1}$ is the Kronecker delta function. These equations hold for $2 \leqq i \leqq N - 1$ if we let $Q_1(\tau) = Q_N(\tau) \equiv 0$. The nonlinear ordinary differential-equation initial-value problem given by (17) and (19) represents the spatial discretization of (13) and must now be solved for the $Q_j(\tau)$, $2 \leqq j \leqq N - 1$.

We use a fully implicit finite difference scheme in time (backward Euler). Let

$$Q_j^n = Q_j(n\Delta\tau) \quad (20)$$

for some choice of $\Delta\tau > 0$. We then let $\dot{Q}_j(n\Delta\tau)$ be approximated by $(Q_j^{n+1} - Q_j^n)/\Delta\tau$ and set $Q_j = Q_j^{n+1}$, $\psi_j = \psi_j^{n+1}$ in (19). On rearranging, we obtain the fully implicit, first-order, finite-difference scheme for solving (19) in time:

$$\begin{aligned}T_{i1}^{n+1}Q_{i-1}^{n+1} + T_{i2}^{n+1}Q_i^{n+1} + T_{i3}^{n+1}Q_{i+1}^{n+1} + A_i(Q_i^{n+1} - Q_{i-1}^{n+1})^2 \\ - A_{i+1}(Q_{i+1}^{n+1} - Q_i^{n+1})^2 = R_i^{n+1}, \quad (21)\end{aligned}$$

where

$$T_{i1}^{n+1} = -\beta/h_i + (\psi_{i-1}^{n+1} + 2\psi_i^{n+1})/6 + h_i/(6\Delta\tau), \quad (22a)$$

$$\begin{aligned}T_{i2}^{n+1} = \beta(1/h_i + 1/h_{i+1}) + (\psi_{i+1}^{n+1} - \psi_{i-1}^{n+1})/6 + (h_i + h_{i+1})/(3\Delta\tau) \\ + \delta_{i,N-1}Q_T/(h_N)^2, \quad (22b)\end{aligned}$$

$$T_{i3}^{n+1} = -\beta/h_{i+1} - (\psi_{i+1}^{n+1} + 2\psi_i^{n+1})/6 + h_{i+1}/(6\Delta\tau), \quad (22c)$$

$$A_i = 1/(2h_i^2), \quad (22d)$$

$$\begin{aligned}R_i^{n+1} = \delta_{i,N-1}[Q_T^2/(2h_N^2) + Q_T(\beta/h_N + \psi_{N-1}^{n+1}/3 + \psi_N^{n+1}/6)] \\ + (h_iQ_{i-1}^n + 2(h_i + h_{i+1})Q_i^n + h_{i+1}Q_{i+1}^n)/(6\Delta\tau). \quad (22e)\end{aligned}$$

Equations (21) hold for $2 \leqq i \leqq N - 1$, $n = 0, 1, 2, \cdots$, with the assumption that $Q_1^n = Q_N^n = 0$, $n = 0, 1, 2, \cdots$ and with the initial conditions $Q_i^0 = Q(y_i, 0)$, $2 \leqq i \leqq N - 1$.

We now find the solution of the nonlinear system of eqs. (21) for fixed n by an iterative Newton method. We drop the superscript n denoting the time step, and for fixed n denote by $Q_i(m)$, $2 \leqq i \leqq N - 1$, the mth iterate of the solution of (21). To obtain $Q_i(m + 1)$ from $Q_i(m)$,

we set $Q_i(m+1) = Q_i(m) + r_i(m)$, substitute this into (21), and linearize the resulting equations for the $r_i(m)$:

$$\begin{aligned}
&\{T_{i1} - 2A_i[Q_i(m) - Q_{i-1}(m)]\}r_{i-1}(m) \\
&\quad + \{T_{i3} - 2A_{i+1}[Q_{i+1}(m) - Q_i(m)]\}r_{i+1}(m) \\
&\quad + \{T_{i2} + 2A_i[Q_i(m) - Q_{i-1}(m)] \\
&\qquad\qquad + 2A_{i+1}[Q_{i+1}(m) - Q_i(m)]\}r_i(m) \\
&= R_i - \{T_{i1}Q_{i-1}(m) + T_{i2}Q_i(m) + T_{i3}Q_{i+1}(m) \\
&\qquad + A_i[Q_i(m) - Q_{i-1}(m)]^2 - A_{i+1}[Q_{i+1}(m) - Q_i(m)]^2\}. \qquad (23)
\end{aligned}$$

These equations hold for $2 \leqq i \leqq N-1$ with $r_1 = r_N = 0$. This is a tridiagonal system of linear equations. Reference 15 contains a concise analysis and very efficient method of solution for such a system of tridiagonal equations.

In practice, the initial estimate of the solution Q_i^{n+1} to (21) is taken to be Q_i^n from the previous time step. So, if $\Delta\tau$ is chosen sufficiently small, the Newton sequence generated by (23) should converge and do so quickly.

What we have described so far is a method for discretizing (9) and (10) in space and time, giving the nonlinear system of eqs. (21), and we have proposed an iterative scheme, given in (23), for solving (21) at each time step. In the next section, we study the feasibility and accuracy of the method.

IV. EXISTENCE AND ACCURACY

We shall show that iteration (23) can be carried out as long as the following conditions are satisfied:

$$0 \leqq Q_2^n \leqq Q_3^n \leqq \cdots \leqq Q_{N-2}^n \leqq Q_{N-1}^n \leqq Q_T, \quad n = 0, 1, 2, \cdots, \qquad (24)$$

$$\sup_{[y_{i-1}, y_i] \times [0, \infty]} |\psi(y, \tau)| \leqq \frac{2\beta}{h_i}, \qquad 2 \leqq i \leqq N. \qquad (25)$$

These conditions are sufficient to ensure the existence of a solution of eqs. (23) for each n. We have not proved it, but in practice they also seem to be necessary. These conditions do not show that the iteration (23) must converge, merely that it is well defined. In fact, if the initial estimate of the solution of (21) is too far off, then in practice the Newton sequence given by (23) may well not converge, and it is necessary to choose $\Delta\tau$ smaller so that Q_i^n provides a better estimate of Q_i^{n+1}.

The monotonicity condition (24) on Q_i^n is merely a necessary consequence of the definition (9) of Q_i^n, since $w(\xi, \tau) \geqq 0$ by definition. The mesh restriction (25), however, is apparently new and fundamental. In practice, if (25) is violated, even at only one point and by a "small"

amount, the solution produced, if any, is highly erratic and non-monotone, and may even be negative.

We now prove that conditions (24) and (25) imply that the matrix of eqs. (23) is strictly diagonally dominant.[16] From this, we can conclude that the matrix has an inverse,[16] so the equations have a solution. From (22a) to (22c) and (25), we see that

$$T_{i1} + T_{i2} + T_{i3} = (h_i + h_{i+1})/(2\Delta\tau) > 0, \tag{26}$$

and

$$\begin{aligned} T_{i2} &\geqq (h_i + h_{i+1})/(3\Delta\tau) > 0; \\ T_{i1} \leqq h_i/(6\Delta\tau), &\qquad T_{i3} \leqq h_{i+1}/(6\Delta\tau). \end{aligned} \tag{27}$$

Because of the monotonicity property (24) and the fact that $T_{i2} > 0$, it is easy to show that

$$\Delta T_i = T_{i2} - |T_{i1}| - |T_{i3}| > 0 \tag{28}$$

implies the diagonal dominance of (23):

$$\begin{aligned} |T_{i2} + 2A_i[Q_i(m) - Q_{i-1}(m)] + 2A_{i+1}[Q_{i+1}(m) - Q_i(m)]| \\ > |T_{i1} - 2A_i[Q_i(m) - Q_{i-1}(m)]| \\ + |T_{i3} - 2A_{i+1}[Q_{i+1}(m) - Q_i(m)]|. \end{aligned} \tag{29}$$

To show that (28) is true, we consider the four possible sign combinations of T_{i1} and T_{i3} and use (26) and (27):

(*i*) $T_{1i} > 0$, $T_{i3} > 0$.

$$\begin{aligned} \Delta T_i = T_{i2} - T_{i1} - T_{i3} &= (h_i + h_{i+1})/(2\Delta\tau) \\ &\quad - 2(T_{i1} + T_{i3}) \geqq (h_i + h_{i+1})/(6\Delta\tau) > 0. \end{aligned}$$

(*ii*) $T_{i1} > 0$, $T_{i3} < 0$.

$$\begin{aligned} \Delta T_i = T_{i2} - T_{i1} + T_{i3} &= (h_i + h_{i+1})/(2\Delta\tau) \\ &\quad - 2T_{i1} \geqq \frac{h_i}{6\Delta\tau} + \frac{h_{i+1}}{2\Delta\tau} > 0. \end{aligned}$$

(*iii*) $T_{i1} < 0$, $T_{i3} > 0$.

$$\begin{aligned} \Delta T_i = T_{i2} + T_{i1} - T_{i3} &= (h_i + h_{i+1})/(2\Delta\tau) \\ &\quad - 2T_{i3} \geqq \frac{h_i}{2\Delta\tau} + \frac{h_{i+1}}{6\Delta\tau} > 0. \end{aligned}$$

(*iv*) $T_{i1} < 0$, $T_{i3} < 0$.

$$\Delta T_i = T_{i2} + T_{i1} + T_{i3} = (h_i + h_{i+1})/(2\Delta\tau) > 0.$$

This completes the proof of the diagonal dominance of (23).

We now discuss the accuracy of the spatial and time discretizations. It is well known (see Ref. 11) that the Galerkin procedure, using chapeau functions, is accurate to $0(h^2)$, where $h = \max_i h_i$ and $0(h^2)/h^2$ represents roughly an upper bound on $Q_{yy}(y, \tau)$ over $[0, 1] \times [0, \infty)$.

We shall not go into the proof of such results here. Rather, a heuristic but useful analysis of the error is presented. The $0(h^2)$ accuracy, basically, comes from the fact that replacing $Q(y, \tau)$ by its interpolant,

$$\sum_{i=1}^{N-1} Q(y_i, \tau) f_i(y) + Q_T f_N(y),$$

results in such a $0(h^2)$ error by using Taylor's theorem on each of the intervals $[y_i, y_{i+1}]$, $i = 1, \cdots, N-1$. A similar statement can be made about $\psi(y, \tau)$ and its interpolant. For the sake of clarity, assume that the mesh is uniform with $h_i \equiv h$, $i = 2, \cdots, N$. Then standard finite difference arguments show that (18) is a spatial finite difference approximation to a function $Q^*(y, \tau)$ obeying

$$Q^*_\tau = Q^*_{yy}(\beta + Q^*_v) - \psi Q^*_y + 0(h^2), \tag{30}$$

where 0 involves terms of the form Q^*_{yy} and its higher-order derivatives, $\partial^{m+n}/\partial y^m \partial \tau^n$. Then, intuitively speaking, since $Q(y, \tau)$ solves (30) to within $0(h^2)$ and $Q^*(y, 0) - Q(y, 0) = 0(h^2)$, we must have $Q^*(y, \tau) - Q(y, \tau) = 0(h^2)$.

Even though (30) is based on the assumption that the spatial mesh is uniform, it shows clearly that the h_i must be small in any region where any of the derivatives $(\partial^{m+n}/\partial y^m \partial \tau^n) Q_{yy}$ are large. Physically, such regions are precisely those regions where the field $\psi(y, \tau)$ is large. This makes restriction (25) quite reasonable, since (25) requires a smaller spatial mesh where the field ψ is large. In fact, we can estimate the number of points N_v, required by (25), using a variable mesh, in a potential rise of v volts: (25) requires that ψ change by no more than $2\beta \cong 1/20$ (at room temperature) over any mesh interval. Then, for example, a potential rise of 5 volts will have $\cong$100 points y_i modeling it. So (25) itself forces a fairly accurate representation of ψ and hence, indirectly, of Q.

However, the time mesh is another matter altogether. The time difference scheme is only first-order accurate and the local time behavior of Q near large values of ψ is rather bad. Thus, application of (21) to (23) alone to solve the problem gives rather poor results. For this reason, we have used polynomial extrapolation to the limit of the results of the first-order scheme (23). A brief discussion of the extrapolation process is given in Appendix C. Ironically, polynomial extrapolation was used because rational extrapolation converged so quickly to the solution that it led to very large $\Delta\tau$ choices (see Ref. 17 for the $\Delta\tau$ monitoring mechanism) which, in turn, led to iteration (23) not converging or taking a very long time doing it. So, even though

polynomial extrapolation is "slower" than rational, it is "better" for our purpose here.

V. CALCULATION OF $Q(y, \infty)$

In most cases of interest, the initial condition for (10) is chosen as an equilibrium solution $Q(y, \infty)$ corresponding to a time-independent potential $\Phi(y)$. It is convenient in these cases to solve for the corresponding $w(y, \infty) = w(y)$ and then integrate to get $Q(y, \infty)$.

Setting $w_\tau = 0$ in (8) yields $0 = [(w + \beta)w_y + w\Phi_y]_y$, which, when integrated twice from 0 to y with the aid of the boundary condition $J(0, \infty) = 0$, yields

$$F(w) = w + \beta \ln \frac{w}{C_0} + \Phi(y) = 0 \tag{31}$$

for some constant C_0. Let y_0 be any point in $[0, 1]$ such that $w(y_0) > 0$. Then

$$C_0 = w(y_0) \exp\left(\frac{\Phi(y_0) + w(y_0)}{\beta}\right). \tag{32}$$

Thus, given $\Phi(y)$ and a single value of $w(y_0) > 0$, the entire equilibrium distribution $w(y)$ is determined. Note that $w(y) > 0$ whenever $\Phi(y)$ is finite.

To find $w(y)$ from (31) we use Newton's method. An initial guess at the solution $w^{(0)}(y) > 0$ is made. The solution is then iterated, the $(n + 1)$th iterate being related to the nth by

$$w^{(n+1)}(y)\left\{1 + \frac{\beta}{w^{(n)}(y)}\right\} = \Phi(y) + \beta\left\{1 - \ln\left(\frac{w^{(n)}(y)}{C_0}\right)\right\}. \tag{33}$$

Since $F'(w) = 1 + \beta/w > 0$ and $F''(w) = -\beta/w^2 < 0$, we see that $F(w)$ is a concave, monotone-increasing function for $w > 0$. Thus, the Newton sequence generated by (33) will converge to the solution (31) no matter what initial $w^{(0)}(y) > 0$ is chosen.

Once the $w(y_i)$, y_i in the Galerkin net $\{y_1, \cdots, y_N\}$ are found using (33), $Q(y_i)$ may be found by the trapezoidal rule for integration. This is consistent with the representation of Q by the chapeau functions, $\bar{Q}$, since the trapezoidal rule is exact for chapeau functions.

VI. ATTEMPTS THAT FAILED

The first attempt at solving (10) was via the finite difference scheme of Ref. 3. It was impractical because the spatial mesh restriction (25) appeared there, also, forcing the spatial mesh to be very small in some regions, although it could be quite large in others. Since any nonuniformity of mesh size in a central finite difference scheme leads to

only first-order accuracy, we were then left with a very fine mesh over the entire interval [0, 1]. This required tens of thousands of points in the spatial mesh, far too many to be practical.

After going to Galerkin's method in space, which has second-order accuracy even with a nonuniform mesh, the solution of (19) posed another problem: It is an extremely "stiff" system of ordinary differential equations, with the coefficients A_i ranging typically from 10^4 to 10^{10}. This is a reflection of the locally quick time and spatial changes in $Q(y, \tau)$ when ψ is large, this fact being transmitted to the h_i by (25). For this reason, any attempt to linearize (19) between time steps for a finite difference scheme in time led to failure—the solution is nowhere near linear over reasonable time intervals when ψ is large. The symptom of this problem, in practice, was that the $\Delta\tau$ required in the polynomial or rational extrapolation process for these linearized schemes was extraordinarily small, requiring in one case more than 10^{10} time steps to cope with a single 5-volt potential swing.

Once a nonlinear approach to the solution of (19) was recognized as probably the only route left, the most obvious "accurate" scheme to use is a fully nonlinear Crank-Nicholson solution of (19). A small digression on this scheme in a simple case is useful here. For the linear system of ordinary differential equations,

$$\mathbf{u}' = \mathbf{A}\mathbf{u}, \tag{34}$$

where $\mathbf{u}$ is a vector and $\mathbf{A}$ a matrix, the Crank-Nicholson approximation to the true solution, $\mathbf{u} = e^{\mathbf{A}\tau}\mathbf{u}_0$, is

$$\mathbf{u}(n\Delta\tau) \cong (\mathbf{I} + \tfrac{1}{2}\mathbf{A}\Delta\tau)^n(\mathbf{I} - \tfrac{1}{2}\mathbf{A}\Delta\tau)^{-n}\mathbf{u}_0.$$

This is based on the approximation[18]

$$e^{\mathbf{A}\Delta\tau} \cong (\mathbf{I} + \tfrac{1}{2}\mathbf{A}\Delta\tau)(\mathbf{I} - \tfrac{1}{2}\mathbf{A}\Delta\tau)^{-1}. \tag{35}$$

Letting $\mathbf{u}(n\Delta\tau) = (u_1^n, \cdots, u_N^n)^T$, this corresponds to the standard finite difference formulation of the Crank-Nicholson scheme:

$$(u_j^{n+1} - u_j^n)/\Delta\tau = \tfrac{1}{2}(\mathbf{A}\mathbf{u}^{n+1} + \mathbf{A}\mathbf{u}^n)_j, \quad 1 \leqq j \leqq N.$$

A nonlinear generalization of the above scheme for (19) would have an error of the form $C(\Delta\tau)^2$; however, C is very large. This is most easily seen by considering (35) for real $A\Delta\tau$ very large (positive or negative). That relation then states that $e^{A\Delta\tau} \cong -1$, which is an exceedingly bad approximation. For a "stiff" system, (34) [or (19)], one that has a wide spread in its eigenvalues for A, the above reasoning indicates that the Crank-Nicholson scheme would give very poor results unless $\Delta\tau$ is very small. In practice, as before, the symptom of

this problem was very small $\Delta\tau$ choices by the extrapolation routines—the same problem that would have required 10^{10} time steps in a linear scheme would have required "only" 10^8 with Crank-Nicholson. (In this matter, see also Ref. 19.)

In all, more than 12 different schemes were programmed and tested on this problem, (9) and (10), with the result that only the one described in Sections II to V is effective for the wide range of ψ distributions required to model both surface and buried-channel CCDs.

VII. ACKNOWLEDGMENTS

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APPENDIX A

In this appendix, we derive eq. (1), the fundamental equation of the Strain-Schryer model, for the case of a BCCD. We choose coordinates as shown in Fig. 3; the x-axis is parallel to the oxide-semiconductor interface and the z-axis is directed into the semiconductor. The potential in the oxide is $\varphi_0(x, z)$ and the potential in the semiconductor is $\varphi_1(x, z)$. The permittivity of the oxide is ϵ_{ox}, that of the semiconductor ϵ_s, and the thickness of the oxide is δ.

In the special case where all the properties of the BCCD are independent of x, the potential in the presence of the inserted charge q has been calculated by Kent[20] and Schryer.[21] They showed that the value of the potential at its minimum in the buried channel is approximately a linear function of the charge q, $\varphi_1 = S_0 q + V_0$, for all values

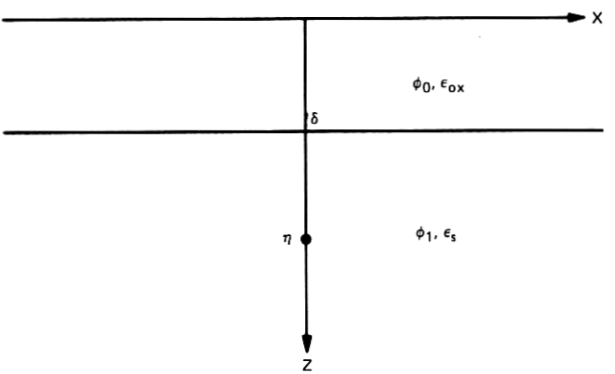

Fig. 3—Coordinate system involved in calculating the potential of a line charge.

of q in the operating range of the device. The elastance S_0 and V_0 are independent of q but depend on the oxide thickness δ and the semiconductor doping, and V_0 also depends strongly on the electrode potential.

In the general case, the Strain-Schryer model assumes that the field in the x-direction in the channel can be approximated by the sum of two terms. The first term is obtained from the above expression for φ_1 by assuming q a function of x and differentiating,

$$E_{x1} = -S_0 \frac{\partial q}{\partial x}. \tag{36}$$

The second term takes into account the field at x resulting from the charge at other points x' in the channel. Because of the metallic electrodes, the charge at x' will induce image charges that will tend to shield the field at x. For this purpose, we first calculate the potential of a unit line charge located at $x = 0$, $z = \eta > \delta$ in the semiconductor. The plane $z = 0$ is assumed to be a perfect conductor at zero potential, and the oxide and semiconductor are assumed uniform. We can write down a solution of Laplace's equation in the form

$$\varphi_0(x, z; \eta) = \int_{-\infty}^{\infty} r(\alpha) \frac{\sinh|\alpha| z}{|\alpha|} e^{i\alpha x} d\alpha, \quad 0 \leqq z \leqq \delta, \tag{37}$$

$$\varphi_1(x, z; \eta) = -\frac{1}{4\pi\epsilon_s} \Psi(x, z; \eta) + \int_{-\infty}^{\infty} s(\alpha) e^{-|\alpha|(z-\delta)} e^{i\alpha x} d\alpha, \quad \delta \leqq z < \infty, \tag{38}$$

where

$$\Psi(x, z; \eta) = \ln \{x^2 + (z - \eta)^2\} - \ln \{x^2 + (z + \eta)^2\}. \tag{39}$$

The function $\Psi(x, z; \eta)$ has the correct singular behavior at $x = 0$, $z = \eta$ and is harmonic everywhere else in $-\infty < x < \infty$, $\delta \leqq z < \infty$. The boundary condition $\varphi_0(x, 0; \eta) = 0$ is satisfied, and the unknown functions $r(\alpha)$ and $s(\alpha)$ must be chosen so that the boundary conditions

$$\varphi_0(x, \delta; \eta) = \varphi_1(x, \delta; \eta), \quad \epsilon_{ox} \frac{\partial \varphi_0}{\partial z}(x, \delta; \eta) = \epsilon_s \frac{\partial \varphi_1}{\partial z}(x, \delta; \eta) \tag{40}$$

are satisfied. It is straightforward to show that

$$\Psi(x, \delta; \eta) = -2 \int_{-\infty}^{\infty} e^{-\eta|\alpha|} \frac{\sinh|\alpha|\delta}{|\alpha|} e^{i\alpha x} d\alpha, \tag{41}$$

$$\frac{\partial \Psi}{\partial z}(x, \delta; \eta) = -2 \int_{-\infty}^{\infty} e^{-\eta|\alpha|} \cosh|\alpha|\delta e^{i\alpha x} d\alpha. \tag{42}$$

If we substitute (37), (38), (41), and (42) into (40), and Fourier-

transform with respect to x, we obtain two linear equations for $r(\alpha)$ and $s(\alpha)$. The solution of these two equations yields

$$r(\alpha) = \frac{1}{\pi} e^{-(\eta-\delta)|\alpha|}\{(\epsilon_{ox} + \epsilon_s)e^{|\alpha|\delta} + (\epsilon_{ox} - \epsilon_s)e^{-|\alpha|\delta}\}^{-1}, \tag{43}$$

$$s(\alpha) = \frac{\sinh|\alpha|\delta}{|\alpha|}\left\{r(\alpha) - \frac{1}{2\pi\epsilon_s} e^{-\eta|\alpha|}\right\}. \tag{44}$$

On substituting (43) and (44) into (37) and (38), we obtain the desired result. If we expand $r(\alpha)$ and $s(\alpha)$ in powers of $e^{-|\alpha|\delta}$, the Fourier integrals can be evaluated, and we can express the potential as the potential resulting from an infinite array of image charges. Since this result is not needed, we do not give it here.

In the buried-channel case, we need the potential resulting from a two-dimensional charge distribution. Let the density of this distribution be $\rho(\xi, \eta)$. Then $q(x) = \int \rho(x, \eta)d\eta$ is the charge appearing in eq. (36). Since the potential resulting from the image charges induced by a line charge at (ξ, η) in the semiconductor is $\varphi(x - \xi, z; \eta)$, we can now write down the second term of the field in the channel as

$$E_{x2} = -\int\int \frac{\partial \varphi_1}{\partial x}(x - \xi, z; \eta)\rho(\xi, \eta)d\xi d\eta. \tag{45}$$

From (38) and (39),

$$\frac{\partial \varphi_1}{\partial x}(x - \xi, z; \eta) = -\frac{1}{2\pi\epsilon_s}\left[\frac{x - \xi}{(x - \xi)^2 + (z - \eta)^2} - \frac{(x - \xi)}{(x - \xi)^2 + (z + \eta)^2}\right] + i\int_{-\infty}^{\infty} \alpha s(\alpha)e^{-|\alpha|(z-\delta)}e^{i\alpha(x-\xi)}d\alpha. \tag{46}$$

Since $(\partial\varphi_1/\partial x)(x - \xi, z; \eta)$ is singular at $\xi = x$, $\eta = z$, the main contribution to the integral in (45) occurs at this point. We expand $\rho(\xi, \eta)$ in a Taylor series about x, keep only the linear terms in the expansion, and extend the limits of the ξ integral from $-\infty$ to ∞. Since $(\partial\varphi_1/\partial x)(x - \xi, z; \eta)$ is an odd function of $x - \xi$, the term involving $\rho(x, \eta)$ vanishes. A straightforward calculation shows that the remaining term is

$$-\frac{1}{2\epsilon_s}\frac{\partial}{\partial x}\int (z + \eta - |z - \eta|)\rho(x, \eta)d\eta - \delta\left(\frac{1}{\epsilon_{ox}} - \frac{1}{\epsilon_x}\right)\frac{\partial q}{\partial x}. \tag{47}$$

The first integral can be transformed by the mean value theorem: $\int (z + \eta - |z - \eta|)\rho(x, \eta)d\eta = (z + \bar{\eta} - |z - \bar{\eta}|)q(x)$, where $\bar{\eta}$ is a point in the interval of integration. In many cases, it is reasonable to

replace the factor $z + \bar{\eta} - |z - \bar{\eta}|$ by a constant $2l$, independent of z. For such cases, we have

$$E_{x2} = -\left\{l/\epsilon_s + \delta\left(\frac{1}{\epsilon_{ox}} - \frac{1}{\epsilon_s}\right)\right\}\frac{\partial q}{\partial x}. \tag{48}$$

If we combine (36) and (48) we obtain (1), where

$$S = S_0 + (l - \delta)/\epsilon_s + \delta/\epsilon_{ox}. \tag{49}$$

Here S_0 must be obtained from a one-dimensional charge-insertion calculation,[20,21] and l must be estimated from the above formulas.

It should be noted that, if we let $\rho(\xi, \eta) = \rho(\xi)D(\eta - \delta)$ in the previous derivation, where $D(x)$ is the Dirac delta function, and set $y = \delta$, we should get the result of Ref. 3 for a surface device. However, in this case, (47) yields δ/ϵ_{ox} for the correction term, while in Ref. 3 the correction term is $2\delta/(\epsilon_s + \epsilon_{ox})$ [eq. (4)]. This is because, in Ref. 3, in the expansion of the field in terms of image charges, only the first image was taken into account.

APPENDIX B

In this appendix, we list several results concerning the chapeau functions $f_j(y)$:

$$\begin{aligned} f_j(y) &= 0, \qquad 0 \leqq y \leqq y_{j-1}, \\ &= (y - y_{j-1})/h_j, \qquad y_{j-1} \leqq y \leqq y_j, \\ &= (y_{j+1} - y)/h_{j+1}, \qquad y_j \leqq y \leqq y_{j+1}, \\ &= 0, \qquad y_{j+1} \leqq y \leqq 1, \end{aligned} \tag{50}$$

where $h_j = y_j - y_{j-1}$.

We list here a number of elementary integrals that are needed in obtaining eqs. (19) from eqs. (18).

$$\int_0^1 (f_j')^2 dy = 1/h_j + 1/h_{j+1}, \tag{51}$$

$$\int_0^1 f_j' f_{j+1}' dy = -1/h_{j+1}, \tag{52}$$

$$\int_0^1 (f_j)^2 dy = (h_{j+1} + h_j)/3, \tag{53}$$

$$\int_0^1 f_j f_{j+1} dy = h_{j+1}/6, \tag{54}$$

$$\int_0^1 (f_j')^3 dy = (h_j)^{-2} - (h_{j+1})^{-2}, \tag{55}$$

$$\int_0^1 (f_j')^2 f_{j+1}' dy = (h_{j+1})^{-2}, \tag{56}$$

$$\int_0^1 (f_j')^2 f_{j-1}' dy = -(h_j)^{-2}, \tag{57}$$

$$\int_0^1 (f_j)^2 f_j' dy = 0, \tag{58}$$

$$\int_0^1 (f_{j+1})^2 f_j' dy = -\tfrac{1}{3}, \tag{59}$$

$$\int_0^1 f_j f_j' f_{j+1} dy = -\tfrac{1}{6}, \tag{60}$$

$$\int_0^1 (f_j)^2 f_{j+1}' dy = \tfrac{1}{3}, \tag{61}$$

$$\int_0^1 f_j f_{j+1}' f_{j+1} dy = \tfrac{1}{6}. \tag{62}$$

In all these expressions, $f_j' = df_j/dy$.

APPENDIX C

In this appendix, we give a brief description of the extrapolation method for solving eqs. (19) in time. We used a linearized, backward Euler method for solving (19) in time. It is first-order accurate. That is, by using a time step of Δt to go from t_0 to $t_1 = t_0 + m\Delta t$, the resulting error at t_1 is $0(\Delta t)$. See either Ref. 22 or Ref. 23 for the proof of such results.

However, much much more is known about these methods. In fact, Stetter[24] has shown, in a very general setting, that processes such as the above backward Euler technique give rise to expansions of the form

$$\mathbf{T}(\Delta t) = \mathbf{T}(0) + \sum_{j=1}^{\infty} \boldsymbol{\tau}_j (\Delta t)^j, \tag{63}$$

where, for our problem, $\mathbf{T}(\Delta t)$ is the value of the vector $(Q_1^m, \cdots, Q_N^m)^T$, which is the value of our approximate solution at $t_1 = t_0 + m\Delta t$, and the $\boldsymbol{\tau}_j$ are vectors that depend only upon t_0 and t_1. Thus, as $\Delta t = (t_1 - t_0)/m$ goes to zero or, equivalently, as m goes to infinity, $\mathbf{T}(\Delta t)$ not only converges, with error $0(\Delta t)$, to the true solution at t_1, namely, $\mathbf{T}(0)$, but each component of $\mathbf{T}(\Delta t)$ looks more and more like a polynomial in Δt. The process of extrapolation consists of simply computing several values, $\mathbf{T}(\Delta t)$, $\mathbf{T}(\Delta t/2)$, $\cdots$, $\mathbf{T}(\Delta t/p)$, and then passing a polynomial of degree $p - 1$ through these data points corresponding to each component. The value of these interpolating polynomials at the origin is the solution $\mathbf{T}(0)$, plus terms of order $(\Delta t)^p$. Here p is called the level of extrapolation.

By using polynomial extrapolation to the limit of the result of the first-order scheme (21), we generate a process that has an error of $0[(\Delta t)^p]$ when p levels of extrapolation are used. This extrapolation process is very well described in Ref. 25, and its application to the numerical solution of ordinary differential equations is also very well described in Ref. 17. It must be stressed that the underlying process, Gragg's modified midpoint rule, which Bulirsch and Stoer extrapolate in Ref. 17, is *not* the one we are proposing to extrapolate here. That rule is second-order accurate and is actually unstable if the equations being solved are stiff. The first-order, linearized, backward Euler method we use here is highly stable under extrapolation, even for very stiff systems like (19). So Ref. 17 should be read with an eye to using extrapolation in solving ordinary differential equations and not to those peculiarities that Bulirsch and Stoer introduce to take special advantage of the nice properties of Gragg's modified midpoint rule. The same technique we have used here to solve (13) was used in Ref. 26 to solve a similar system. It is of interest that, for both these problems, polynomial extrapolation was found to be 15 to 20 percent faster than rational extrapolation. This is in contrast to the finding in Ref. 17 that rational extrapolating is usually the faster of the two, at least when extrapolating Gragg's modified midpoint rule.

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