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MODELING OF HIGH CURRENT INJECTION INTO BIPOLAR SEMICONDUCTORS.(U)

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MODELING OF HIGH CURRENT INJECTION INTO BIPOLAR SEMICONDUCTORS

October 1977

Final Report

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AIR FORCE WEAPONS LABORATORY
Air Force Systems Command
Kirtland Air Force Base, NM 87117

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This technical report has been reviewed and is approved for publication.

Edward O. Fuller

EDWARD O. FULLER
Captain, USAF
Project Officer

FOR THE COMMANDER

Aaron B. Loggins

AARON B. LOGGINS
Lt Colonel, USAF
Chief, Phenomenology and Technology Branch

James L. Griggs Jr.

JAMES L. GRIGGS, JR.
Colonel, USAF
Chief, Electronics Division

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Two techniques were used in an attempt to solve the problem of high current injection into a bipolar semiconductor. The first technique was by finite differences, and the second was by the method of lines. Because of the physical model chosen for the system, neither method would converge. An extended bibliography is included.

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PREFACE

Most researchers have used finite differences with nonlinear scaling to solve the problem of high current injection into bipolar devices. This report records an attempt to solve the same problems with another technique and resolve the problems with fewer restrictions than have been used previously.

Chris Ashley, Roe J. Maier and A. Brent White of the Electronics Division, Air Force Weapons Laboratory (AFWL), have provided much useful information necessary for the work reported in this report. Dr. Donald C. Wunsch (AFWL/EL) provided invaluable assistance in the research efforts of this problem. I wish to thank these individuals for their help.

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SECTION I

INTRODUCTION

This technical report documents the results of an effort to model the effects of high current injection into bipolar semiconductors. The work was started at the recommendation of Dr. Donald C. Wunsch of the Air Force Weapons Laboratory.

When a transistor device experiences an electromagnetic pulse (EMP), high currents and voltages can be induced between the metal contacts of the device. Depending on the materials and doping, significant changes can occur in the distributions of the electric field, the electron density, the "hole" density, and traps (ref. 1). Because of the significant heating of the devices at high current, a temperature dependency was included in the model. The number of spatial dimensions was reduced to one to keep the problem tractable.

Two techniques or models were used in an attempt to solve the above problem. The first technique employed finite differencing in both variables (time and space) and the second was based on reducing the model equations to a system of first order differential equations and then solving this system of equations. Difficulties were encountered in each of the two techniques. In both cases, the difficulties were related to the physical problem. This problem is characterized by very large boundary values which affect the solutions obtained. Because of this problem and others described in this report, no successful predictions were made describing the effects of high current injection.

SECTION II

DERIVATION OF THE MODEL EQUATIONS

Various assumptions are made concerning the special dimensions, the form of the coefficients, and the number of dependent and independent variables. The first assumption is that of one special dimension, say x. Using this assumption, one reduces Maxwell's equations as follows (ref. 2):

$$\text{curl } E = -\frac{\partial B}{\partial t} \tag{1a}$$

$$\text{curl } H = \frac{\partial D}{\partial t} + J \tag{1b}$$

$$\text{div } B = 0 \tag{1c}$$

$$\text{div } D = \rho \tag{1d}$$

$$\text{curl } E = \frac{\partial E}{\partial x}(0, -1, +1) = -\frac{\partial B}{\partial t} \tag{1c}$$

where

$$D(x, t) = \int_{\infty}^{t} \varepsilon(t - t')\, E(X, t')\, dt'$$

$$\text{div } B = \frac{\partial B}{\partial x}$$

$$= 0$$

from the dimensional assumption, then one may conclude that curl H = 0. The next assumption is about the form of the current density J. One usually assumes that the current density takes the form (refs. 3, 4, 5, and 6)

$$J_n = q\mu_n E\, n + q\, D_n \frac{\partial n}{\partial x} = q\, \mu_2\, U^2\, U^6 + q\, D_2 \frac{\partial U^2}{\partial x} \tag{2a}$$

$$J_p = q\mu_p E\, p - q\, D_p \frac{\partial p}{\partial x} = q\, \mu_3\, U^3\, U^6 - q\, D_3 \frac{\partial U^3}{\partial x} \tag{2b}$$

with

$$J = J_n + J_p$$

The quantities μn, μp, n, p, Dn, Dp, q are defined in the glossary of terms; U^1 through U^6 are a relabeling of these variables. Some constants will be relabeled in view of their connection with the various dependent variables.

Since curl H = 0, equation (1b) reduces to the equation

$$\frac{\partial D}{\partial t} = - J_n - J_p$$

$$= q\, D_3 \frac{\partial U^3}{\partial x} - q(\mu_3\, U^3\, U^6 + \mu_2\, U^2\, U^6) - q\, D_2 \frac{\partial U^2}{\partial x}$$

and the generation rates for U^2 and U^3 are given by the equations (refs. 3, 4, 5, and 6)

$$\frac{\partial U^2}{\partial t} = g - \frac{U^2}{\tau_2} + \frac{1}{q}\ \frac{\partial}{\partial x}(J_n) \tag{3a}$$

$$\frac{\partial U^3}{\partial t} = g - \frac{U^3}{\tau_3} - \frac{1}{q}\ \frac{\partial}{\partial x}(J_p) \tag{3b}$$

where $g = g(x, t, u)$, $u = \upsilon\,(u_1, u_2, u_3, u_4, u_5, u_6)$. The terms τ_i are related to the trapping of electrons and holes by the media. The τ_i are simply the average life times of holes and electrons between capture. Substituting equations (2a) and (2b) into equations (3a) and (3b) results in the following:

$$\frac{\partial U^1}{\partial t} = \frac{\partial D}{\partial t} = -q(\mu_3\, U^3\, U^6 + \mu_2\, U^2\, U^6) + q\left(D_2 \frac{\partial U^3}{\partial x} - D_2 \frac{\partial U^2}{\partial x}\right) \tag{4a}$$

$$\frac{\partial U^2}{\partial t} = g - \frac{U^2}{\tau_2} + \frac{\partial}{\partial x}\left(\mu_2\, U^2\, U^6 + D_2 \frac{\partial U^2}{\partial x}\right) \tag{4b}$$

$$\frac{\partial U^3}{\partial t} = g - \frac{U^3}{\tau_3} - \frac{\partial}{\partial x}\left(\mu_3\, U^3\, U^6 - D_3 \frac{\partial U^3}{\partial x}\right) \tag{4c}$$

$$\frac{\partial U^4}{\partial t} = \frac{K}{a}\ \frac{\partial^2 U^4}{\partial x^2} + \left(-U^6(J_n + J_p)\right) \tag{4d}$$

$$\frac{\partial U^5}{\partial t} = - < v_2\ \sigma_2 > U^2\ U^5 + < v_3\ \sigma_3 > (N - U^5)\ U^3 \tag{4e}$$

$$U^1 = \varepsilon U^6 \tag{4f}$$

The equation $U^1 = \varepsilon U^6$ *is an approximation* that is valid at low frequencies and isotropic media. The size of a large bipolar transistor is about one millimeter in its largest dimension. For such a transistor to "see" or sense wave phenomena, the frequency of the wave must be larger than 10^{11} hertz since

$$f = C/\Gamma \simeq (3 \times 10^8\ \text{m/sec})/10^{-3}\ \text{m}$$

$$= 3 \times 10^{11}\ \text{hertz.}$$

This is in the lower range of the region of visible light (near the upper infrared region). This approximation allows one to reduce the number of variables from six to five. The reduced set of equations is as follows:

$$\varepsilon \frac{\partial U^1}{\partial t} = -q(\mu_2\ U^2 + \mu_3\ U^3)\ U^1 + q\left(D_3 \frac{\partial U^3}{\partial x} - D_2 \frac{\partial U^2}{\partial x}\right) \tag{5a}$$

$$\frac{\partial U^2}{\partial t} = g(x,\ t,\ U) - \frac{U^2}{\tau_2} + \frac{\partial}{\partial x}\left(\mu_2\ U^2\ U^1 + D_2 \frac{\partial U^2}{\partial x}\right) \tag{5b}$$

$$\frac{\partial U^3}{\partial t} = g(x,\ t,\ U) - \frac{U^3}{\tau_3} - \frac{\partial}{\partial x}\left(\mu_3\ U^3\ U^6 - D_3 \frac{\partial U^3}{\partial x}\right) \tag{5c}$$

$$\frac{\partial U^4}{\partial t} = \frac{K}{a}\ \frac{\partial^2 U^4}{\partial x^2} - q(U^1)^2\ (\mu_2\ U^2 + \mu_3\ U^3) - qU^1 \left(D_2 \frac{\partial U^2}{\partial x} - D_3 \frac{\partial U^3}{\partial x}\right) \tag{5d}$$

$$\frac{\partial U^5}{\partial t} = - < v_2\ \sigma_2 > U^5\ U^2 - < v_3\ \sigma_3 > U^5\ U^3 + < v_3\ \sigma_3 > N\ U^3 \tag{5e}$$

The terms $< V_j\ \sigma_j >$ *are the average cross sections for the electrons* ($j = 2$) and holes ($j = 3$), i.e., capture possibilities. The D_i are diffusion parameters which depend on the electric field U^1, temperature U^4, and the two concentrations. Equation (5e) controls the number of traps and number of electrons available to the system as a whole, i.e., it gives the system charge conservation.

SECTION III

FINITE DIFFERENCE TECHNIQUE

Finite differences was the first of two techniques by which the solution of equations (5) was effected. This technique makes use of the definition of the partial derivative of a function, i. e.

$$\frac{\partial f}{\partial t}(x, t) = \lim_{h \to 0} \frac{f(x, t+h) - f(x, t)}{h}$$

$$\simeq \frac{f(x, t+h) - f(x, t)}{h}$$

and

$$\frac{\partial f}{\partial x} = \lim_{h \to 0} \frac{f(x+h, t) - f(x, t)}{h}$$

and

$$\frac{\partial^2 f}{\partial x^2} = \lim_{h \to 0} \frac{\frac{\partial f}{\partial x}(x+h, t) - \frac{f}{x}(x, t)}{h}$$

A similar expression holds for $\frac{\partial^2 f}{\partial t^2}$. by partitioning the x-t space, one can step through the time portion of the axes or the spatial axis. The second derivative of f with respect to (say x) is replaced by

$$\frac{\partial^2 f}{\partial x^2} \simeq \frac{f_{j+1,k} - 2 f_{j,k} + f_{j-1,k}}{(\Delta x)^2}$$

where

$$f_{j,k} = f(x_j, t_k)$$

$$x_j = x + j\Delta x$$

$$t_k = t + k\Delta t$$

$$k, j = 1, \cdots M$$

This leads to the following set of explicity equations (note that superscripts refer to the name of the variable and subscripts tell where in the mesh the function is evaluated).

$$U^1_{j,k+1} - U^1_{j,k} = \frac{q\Delta t}{\Delta x} - \left(\mu^2_{j,k}\, U^2_{j,k} + \mu^3_{j,k}\, U^3_{j,k}\right)\Delta x$$

$$+ D^3_{j,k}\left(U^3_{j,k} - U^3_{j-1,k}\right) - D^2_{j,k}\left(U^2_{j,k} - U^2_{j-1,k}\right) \qquad (6a)$$

$$U^2_{j,k+1} - U^2_{j,k} = \Delta t\, g_{j,k} - \frac{U^2_{j,k}}{\tau_2}\Delta t + \frac{\Delta t}{\Delta x}\mu^1_{j,k}\, U^2_{j,k}\left(\mu^2_{j,k} - \mu^2_{j-1,k}\right)$$

$$+ \mu^2_{j,k}\frac{\Delta t}{\Delta x}U^1_{j,k}\left(U^2_{j,k} - U^2_{j-1,k}\right) + U^2_{j,k}\left(U^1_{j,k} - U^1_{j-1,k}\right)$$

$$+ D^2_{j,k}\frac{\Delta t}{\Delta x^2}\left(U^2_{j+1,k} - 2U^2_{j,k} + U^2_{j-1,k}\right)$$

$$+ \frac{\Delta t}{\Delta x^2}\left(D^2_{j,k} - D^2_{j-1,k}\right)\left(U^2_{j,k} - U^2_{j-1,k}\right) \qquad (6b)$$

$$U^3_{j,k+1} - U^3_{j,k} = \Delta t\, g_{j,k} - \frac{U^3_{j,k}}{\tau_3} - \frac{U^1_{j,k}\, U^3_{j,k}}{\Delta x}\ \mu^3_{j,k} - \mu^3_{j-1,k}$$

$$- \frac{\mu^3_{j,k}}{\Delta x}\left(U^1_{j,k} - U^1_{j-1,k}\right)U^3_{j,k} - \frac{\mu^3_{j,k}\, U^1_{j,k}}{\Delta x}\left(U^3_{j,k} - U^3_{j-1,k}\right)$$

$$+ D^3_{j,k}\frac{1}{\Delta x^2}\left(U^3_{j+1,k} - 2\,U^3_{j,k} + U^3_{j-1,k}\right)$$

$$+ \frac{1}{\Delta x^2}\left(U^3_{j,k} - U^3_{j-1,k}\right)\left(D^3_{j,k} - D^3_{j-1,k}\right) \qquad (6c)$$

$$U^4_{j,k+1} - U^4_{j,k} = \frac{K\,\Delta t}{a\,\Delta x^2}\left(U^4_{j+1,k} - 2\,U^4_{j,k} + U^4_{j-1,k}\right) + U^1_{j,k}\left(U^1_{j,k} - U^1_{j,k-1}\right)\Delta t \qquad (6d)$$

$$U^5_{j,k+1} - U^5_{j,k} = - < v_3\,\sigma_3 > U^5_{j,k}\, U^3_{j,k} - < v_2\,\sigma_2 > U^5_{j,k}\, U^2_{j,k}$$

$$+ < v_3\,\sigma_3 > N\, U^3_{j,k} \qquad (6e)$$

which is the explicit formulation of equations (5) and where

$$g_{j,k} = g\left(x_j,\ t_k,\ U^1_{j,k},\ U^2_{j,k},\ U^3_{j,k},\ U^4_{j,k},\ U^5_{j,k},\ U^6_{j,k}\right)$$

$$= g\left(x_j,\ t_k,\ \vec{U}_{j,k}\right)$$

i.e., $u_{jk} = \vec{u}_{jk}$. By explicit, one means that the right hand side of the equation depends on known values at previous mesh points. Richtmeyer and Morton (ref. 7) have shown that under certain circumstances the explicit formulation of finite differences will be unstable. It is possible to rewrite equations (6) so that the system is either implicit or a combination of implicit and explicit as shown for the diffusion equation in reference 8 by introducing a parameter Θ. For example, equation (6d) becomes

$$U^4_{j,k+1} - U^4_{j,k} = \Theta \frac{K\Delta t}{\Delta x^2}\left(U^4_{j+1,k+1} - 2\,U^4_{j,k+1} + U^4_{j-1,k+1}\right)$$

$$+ (1 - \Theta)\left(\frac{K\Delta T}{\Delta x^2}\right)\left(U^4_{j+1,\,k} - 2U^4_{j,k} + U^4_{j-1,k}\right)$$

$$+ U^1_{j,k}\,\Delta t\left(U^1_{j,k+1} - U^2_{j,k}\right) \tag{7}$$

where $\Theta\varepsilon[0,\ 1] \subseteq R$. For $\Theta = 0$ the above explicit formulation is obtained while for $\Theta = 1$, a fully implicit method is obtained. The Crank-Nicholson method is obtained when $\Theta = 1/2$. Ford and others have shown that the truncation error for the diffusion equation using constant coefficients and the Crank-Nicholson method is $0\ \{(\Delta x)^2 + (\Delta t)^2\}$ while the purely implicit technique and explicit techniques give $0\ \{(\Delta x)^2 + (\Delta t)\}$ (refs. 7 and 8). In reference 7, the authors show that for constant coefficients the finite difference scheme is stable for $\Theta\varepsilon\ (1/2,\ 1)$. Lees (ref. 9) has shown that the Crank-Nicholson scheme is stable for certain types of quasi-linear parabolic equations. Lees states that how one differences the lower order terms in the equation

$$\sigma \frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + A_1(x, t)\frac{\partial u}{\partial t} + A_2(x,\ t)\ u(x,\ t)$$

is a matter of truncation error and not stability. There are requirements on σ and u that are needed so that a pure implicit finite difference operator will be stable (namely $\sigma > 0$ and $u \epsilon C^3$). In order to determine whether or not the equations (6) are stable, the coefficients of the equations of second order will have to be analyzed to determine if they satisfy the criteria given by Lees. The first order equations will be inspected at a later time.

The parameters u_i and D_i are the mobilities and diffusion rates of the electrons and holes in the medium. Various forms of equations are used according to some of the hypotheses made by the author of the paper. Maier (ref. 1) reports on using a multitrap model as well as one trap model. Van Lint (ref. 6); Raburn and Causey (ref. 3); Leadon (ref. 4); and Newdeck (ref. 5) all use a variation of the model due to Shockley and Read (ref. 10). These equations take the form

$$\mu_j = \frac{\alpha_j \exp\left(-\beta_j / U^1\right)}{(U^4)} \tag{8a}$$

$$D_j = v_j / U^1 \text{ (or } D_j = \text{constant)} \tag{8b}$$

depending on the author. In many cases the constraints or parameters are curve fitted between experimental data assuming a particular form of variation. The function g is the recombination-generation term which gives the relationship between electron-hole pairs during the generation and recombination processes.

Using the Shockley-Read model (ref. 10), the form of g is (refs. 3, 4, and 5)

$$g(x, t, U) = \frac{N_i - U^2 U^3}{\tau_2 (U^2 + N_i) + \tau_3 (U^3 + N_i)} \tag{9}$$

with

$$N_i = \alpha (U^4)^{3/2} \exp\left(-q(E - E')/(2 K_b U^4)\right)$$

and α constant.

The equations of interest are (6b), (6c), and (6d) or (4b), (4c), and (4d). The coefficients of the lower order terms in equation (6b) are μ_2, μ^6 and $g - \frac{U^2}{\tau_2} + \mu_2 \frac{\partial U^2}{\partial_x} D_2$.

The requirement given by Lees (ref. 9) for the terms A_1, A_2 is that

$$\sup_G \left| A_i(x, t) \right| \leq M$$

but note that these A_i do not depend on the solutions; hence we may not be able to use this theory unless we assume that the terms $\frac{\partial U^2}{\partial x}$, $\frac{1}{\tau_2}$, g and U^2 are all uniformly bounded or constant. In reference 9, Lees requires that the coefficient of the term $\frac{\partial^2 U}{\partial x^2}$ have uniformly bounded partial derivative as well as being uniformly bounded away from zero. If these conditions are satisfied then the equation

$$\frac{\partial u}{\partial t} = \sigma(x, t, u) \frac{\partial^2 u}{\partial x^2}$$

will be unconditionally stable with respect to the norm $||\cdot||$.

SECTION IV

ORDINARY DIFFERENTIAL EQUATION APPROACH

Another technique for solving systems of partial differential equations is discussed by Shampine (ref. 12) for the diffusion equation. Basically, one finite differences the spacial derivatives and steps through in time or finite differences in the time and solves Poisson's equation. The choice depends on how complicated the derivatives are and the form of the resulting matrices. Assuming that one finite differences the spatial variables then equations (4) become

$$\frac{dU_j^1}{dt} = q\left(\mu_3 U_j^1 U_j^3 + \mu_2 U_j^1\ U_j^2\right) + q\left(D_j^3 (U_j{}^3 - U_{j-1}^3) - D_j^2 (U_j^2 - U_{j-1}^2)\right) \frac{1}{\Delta x} \qquad (10a)$$

$$\frac{dU_j}{dt} = g_j - \frac{U_j^2}{\tau_2} + \delta_x(\mu^2\ U^2\ U^1) + \left(\frac{1}{\Delta x}\right)^2 \delta_x \left(D_j^2\right) \delta_x \left(U_j^2\right)$$

$$+ \left(\frac{1}{\Delta x}\right)^2 D_j^2 \left(U_{j+1}^2 - 2\ U_j^2 + U_{j-1}^2\right) \qquad (10b)$$

$$\frac{dU_j^3}{dt} = g_j - \frac{U_j^3}{\tau_3} - \delta_x \left(\mu^3\ U_j^1\ U_j^3\right) + \left(\frac{1}{\Delta x}\right)^2 \delta_x \left(D_j^3\right) \delta_x \left(U_j^3\right) \qquad (10c)$$

$$\frac{dU_j^4}{dt} = (K/a) \left(U_{j+1}^4 - 2\ U_j^4 + U_{j-1}^4\right)/(\Delta x)^2 - U_j^1 \left(\frac{dU_j^1}{dt}\right) \qquad (10d)$$

$$\frac{dU_j^5}{dt} = -\ P_2\ U_j^5\ U_j^2 + P_3 \left(N - U_j^5\ \ U_j^3\right) \qquad (10e)$$

for j = 1, 2, ... M where M is the number of mesh points used to partition the x-interval of interest. The existence of a solution has been given in various books for systems of ordinary differential equations, namely Hille (ref. 13), Caratheordory (ref. 14). The most general conditions for existence are given in reference 14; but, under his assumptions, uniqueness cannot be assured. Stronger assumptions are necessary and these are investigated in reference 13. The equations below provide a very compact method for rewriting equations (10).

$$\frac{dU^1}{dt} = f_1(x, t, U) \tag{11a}$$

$$\frac{dU^2}{dt} = f_2(x, t, U) \tag{11b}$$

$$\frac{dU^3}{dt} + f_3(x, t, U) \tag{11c}$$

$$\frac{dU^4}{dt} = f_4(x, t, U) \tag{11d}$$

$$\frac{dU^5}{dt} = f_5(x, t, U) \tag{11e}$$

$$\vdots$$

with

$$U^j(x, 0) = u_j\ (x)$$

which may be rewritten as

$$U' = f(x, t, U) \tag{12a}$$

$$U(0) = U^0 \tag{12b}$$

Caratheordory states the following theorem (ref. 14):

If the n functions f_i are continuous in a closed and bounded region $\overline{G}$ of an n + 1 dimensional space through each interior point (t^0, u^0) of G, there exists at least one continuously differentiable curve $\chi_i = \chi_i(t)$ which is defined on $|t - t^0| \leq a$ and satisfies equation (12). Since this theory says nothing about uniqueness nor how the solutions depend on the initial conditions nor how the solutions vary when the functions f_i are perturbed, then one usually requires that the function f_i have more stringent conditions. These fall into two classes. The first is concerned with bounding the partial derivatives of the f_i with respect to the U_i and the second is Lipschitz continuity of the function f_i in the U variables. Since f is a vector function in R^{M+1}, one defines its derivative as the linear transformation, say B that satisfies (ref. 15)

$$\lim_{||h||\to 0} \frac{||f(x + h) - f(x) - Bh||}{||h||} = 0$$

if the limit exists and such a transformation B can be found. The symbolization $h \to 0$ implies for $\varepsilon > 0$, $||h|| < 0$ where $h \in R^n$. The matrix B which is the Frechet derivative of f is related to its Jacobian $\left\{\frac{\partial f}{\partial u}\right\}$. A theorem due to Kamke (1930) and to the authors Coddington and Levinson (1955) is as follows (see reference 13):

Let f(x,y) be continuous in the $|x - x_0| \leq a$, $||y - y|| \leq b$ and satisfy $||F(x, z) - F(x, z)|| \leq W\left(|x - x_0|, ||y - y_0||\right)$ where W satisfies the following

1. Let $H(r) = \left\{h \in C^+ [0, t] \mid h(0) = 0, \text{ and } \lim_{t\downarrow 0} \frac{h(t)}{t} = 0\right\}$
2. $W(x, y) \geq 0$
3. If $y_1 > y_2$ then for x_0 fixed, $W(x_0, y_1) \geq W(x_0, y_2)$
4. $\exists c > 0$, such that $W(x, cx) \leq c$, $x \in (0, a)$
5. For $h \in H(r)$ the Lim $W(t, h(t)) = 0$

then the only solution in H(a) of $z' = W(t, z(t))$ is $z(t) \equiv 0$ and $y' = F(x, y)$ has a unique solution passing through (x_0, y_0).

Another theorem is given in Hille (ref. 13) whereby the Lipschitz condition on F is replaced by a condition on its Frechet derivation, that its Frechet derivative exist, be continuous, and be bounded in the domain D. The full theorem (ref. 13) states that in the differential equation $y' = f(x, y)$, $f: R^1 \times R^n \to R^n$, where f is continuous, bounded in $D = \left\{(x, y) \in R \times R^n \mid |x - x_0| \leq a, ||y - y_0|| \leq b\right\}$ i.e., $||f(x, y)|| < M$, for all $(x, y) \in D$, the Frechet derivative exists, is bounded by B', for small values of $||y - y_0||$ we have $f(x, y) - (f, y_0) = \left[\frac{f}{\partial y_i}\right](y - y_0) + O\left(||y - y_0||\right)$ then $\exists!$ solution of $y' = f(x, y)$ passing through $(x_0, y_0) \in D$.

One may obtain a solution to system (10) by assuming those parts of the system due to "diffusion" to be zero. Under these circumstances, the results are as follows:

$$\frac{dU^1}{dt} = -\frac{q}{\varepsilon}\left(\mu_2 U^2 + \mu_3 U^3\right) U^1$$

$$\frac{dU^2}{dt} = g(x, t, U) - \frac{U^2}{\tau_2}$$

$$\frac{dU^3}{dt} = g(x, t, U) - \frac{U^3}{\tau_3}$$

$$\frac{dU^5}{dt} = - P_2 U^5 U^2 + P_3 U^3 (N - U^5)$$

with U^4 being constant throughout the medium. The parameters P_j are then determined from the energies of the electrons and holes where they are assumed to be a Fermi-Dirac gas. Under this formulation, Kittel gives the probabilities for trapping as follows (ref. 11):

$$P_j = 1/\left(1 + \exp\left((E - E_j')/(2\, k_b U^4)\right)\right)$$

where

$$E_j' = \text{constant}\ (U_j^4)^{2/3}$$

with E_j = constant $(U_j)^{2/3}$. These equations were modeled under a system of programs called Extended Sceptre (ref. 16). These routines allow one to solve systems of stiff ordinary differential equations as well as electronic circuits. With only a few cards, one can implement the above system without having to write the integration routines. The implementation used is given in the appendix. Control of the time increment is by SCEPTRE and before going to the next time step the program iterates the solution to obtain a "better" solution. If after a fixed number of tries the program finds nonconvergence, then the program reduces the time step size and redoes the problem with best known data. This type of control is necessary when stiff differential systems are encountered to reduce truncation error as well as round off error (by reducing the number of step calculations). The system also calculates the Jacobian matrix noted above and notes whether the matrix is of full rank or singular.

SECTION V

CONCLUSIONS

There are two problems in solving systems of partial differential equations with finite differences: consistency and stability. The system of equations (4) or (6) exhibited a problem called instability which can radically affect the convergence to a solution. In using a purely explicit formulation, one has to use such small Δt's that the resulting answers for times corresponding to 1000 initial Δt's are almost entirely error because of round off error. This problem was also apparent in the purely implicit formulation because the answers would still not converge. The answers at the second and third steps were grossly in error in both cases (the electric field was given as 10^{26} volts per meter). Thus there was an error in the modeling of the problem and the equations were not consistent, hence convergence would be impossible.

The second technique exhibited a different problem in that SCEPTRE said the matrix B was singular. While it calculated answers for the first time step, no answers were calculated for the second time step. Very small time steps were used so that this would not happen, but no results were forthcoming.

It appears that the linearization used in the second technique does not yield a useful approximation to the original problem. In fact, no approximation is found at all. A more exact approximation to the original equations would perhaps change the singularity of the Jacobian matrix and thus yield a useful approximation to the solution of system (6).

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APPENDIX

LINEAR APPOXIMATION BY ORDINARY DIFFERENTIAL EQUATIONS

```
CIRCUIT DESCRIPTION
$
$       PY1= ELECTRIC FIELD, PY2= ELECTRON CONCENTRATION, PY3= HOLE
$       CONCENTRATION, PY4= TEMPERATURE, PY5= NUMBER OF TRAPS, PY6=
$       INTERNAL ENERGY, PG= RIGHT HAND SIDE IE. FORCING FUNCTION.
$       THIS FORMULATION ASSUMES CONSTANT TEMPERATUR AND FERMI GAS-TYPE
$       LAW FOR CALCULATING CAPTURE PROBABILITIES.
$
DEFINED PARAMETERS
$       INITIALIZE THE CONSTANTS
   PL= 10.E-6
   PEPS= 3.32032E-11
   PQ= 1.602E-19
   PNT= 1.1E23
   PK= 1.38062E-23
   PC= 5.84189E-38
    PEN=0
   PT2=1.E-9
   PT3=1.E-9
$       INITIALIZE THE VARIABLES
   PY1= 1.E6
   PY2=1.E23
   PY3=1.E22
   PY5= .1285713E17
   PY6=0
$       SET UP THE COEFFICIENTS
   PEF= XEF(PC*(PY2*PY2)**(1./3.))
   PEFP= XEFP (PC*(PY3*PY3)**(1./3.))
   PY4= Q1(PEPS,PY1,DPY1)
   PM2= XM2 ((PY4**(-2.5))*(1.436E4)*EXP(-2.555E4/ABS(PY1)))
   PM3= XM3((PY4**(-2.5))*(8.5E4)*EXP(-4.76E4/ABS(PY1)))
   PNI= XNI((3.1623E23)*(PY4**1.5)* EXP(-PQ*(PEF+PEFP)/(2.*PK*PY4)))
   PG= XG(PQ*(PNI*PNI-PY2*PY3)/((PY2+PY3+PNI+PNI)*PT2))
   PFE= XFE(1./(1.+EXP((PEN-PEF)/(PK*PY4))))
   PFP= XFP(1./(1.+EXP((PEN-PEFP)/(PK*PY4))))
$       DEFINE THE DIFFERENTIAL EQUATIONS
   DPY1= X1(-PQ*(PM2*PY2+PM3*PY3)*PY1/PEPS)
   DPY2= X2(PG-(PY2/PT2))
   DPY3= X3(PG-PY3/PT3)
   DPY5= X5(-PFE*PY5*DPY2+PFP*DPY3*(PNT-PY5))
   DPY6= X6(PY6-PL*PY1*DPY1)
FUNCTIONS
   Q1(A,B,C)= (FUN(A,B,C))
OUTPUTS
   PY1,PY2,PY3,PY4,PY5,PY6,PEF,PEFP,PNI,PLOT
   XSTPSZ,DPY1,DPY2,DPY3,DPY5,DPY6
RUNCONTROLS
   MAXIMUM PRINT POINTS= 2000
   COMPUTER TIME LIMIT = 20
   STARTING STEP SIZE= 1.E-40
   MINIMUM STEP SIZE= 1.E-45
    STOP TIME= 50.E-9
   INTEGRATION ROUTINE = XPO
   WRITE SIMULB DATA
SUBPROGRAM
   FUNCTION FUN (A,B,C)
   COMMON /CNTRLS/TIME
   X= A*B*C
   IF (TIME.EQ.0) X=293.16
   FUN=X
   RETURN
   END
```

ABBREVIATIONS AND SYMBOLS

$B = \vec{B}$	magnetic induction
$D = \vec{D} = U^1$	displacement field
$E = U^6 = \vec{E}$	electric fields
$\mathcal{E}$	total energy of the system
$\mathcal{E}'$	energy state of an electron or hole
$H = \vec{H}$	magnetic field
J_n, J_p	electron, hole current densities
K	thermal conductivity
K_b	Boltzman's constant
M	number of mesh points partitioning an interval $[a, b] \subseteq R$
N	total number of traps
P_j, $< v_j \alpha_j >$	probability that an electron, hole, will be captured by a trap
R	the real line
a	thermal diffusivity
f	frequency
$n(U^2)$, $p(U^3)$	electron, hole densities
q	electric charge
$\sup_G \lvert A(x, t)\rvert$	last upper bound of t for all χ in the closure of the set G
t	time
χ_i	curve in space
$\delta_x = f$	first order difference in x of the function $f = f(x) - f(x - \Delta x)$
ε	is an element of permittivity
Γ	wavelength
μ_0	permeability of free space
μ_2, μ_3	electron, hole mobilities
ρ	total electric charge
τ_2, τ_3	electron, hole average lifetimes
$\lVert \quad \rVert$	norm (depends on the space)
$\lvert \cdot \rvert$	Euclidean norm
$\Rightarrow$	implies
$\exists$	there exists
$\exists!$	there exists a unique
$\subseteq$	containment (eg. $A \subseteq B$ for $x \varepsilon A \Rightarrow x \varepsilon B$)