SENSITIVITY ANALYSIS AND ITS APPLICATION IN THE OPTIMUM
DESIGN OF SEMICONDUCTOR DEVICES

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ABSTRACT

The calculation of design sensitivities form the central
operation in many optimisation problems. When the behaviour
of the system is nonlinear it becomes essential to development
cost effective algorithms to compute these derivatives. This
is particularly important when applying such procedures to the
design of semiconductors due to the highly nonlinear behaviour
exhibited. A technique is developed for calculating sensitiv-
ities through operating on the converged solution of a set of
equations which have been solved by the finite element method.
Comparisons are made between numerical results and known analyt-
ical solutions for quasi-harmonic applications. Applications
to the design of off-state p-n junctions are also described.

1. INTRODUCTION

Semiconductor design in many cases is based on the usual
engineering approach that if a satisfactory or otherwise reason-
able solution has been found then the design stage can be term-
inated. During the last few years there has been considerable
research activity in the numerical solution of the equations
governing potential distributions in semiconductor devices [1]
[2] and this has lead to the accurate solution of device response.
With such powerful numerical solutions available it becomes
immediately apparent that device response can be examined in
depth at the design stage and furthermore the possibility of
applying optimisation techniques can be explored. For instance
device configurations, material properties and terminal contact
positions could be considered as design parameters. The opti-
misation problem could then be posed as find the set of parameters
which minimise some particular device response within the limits
of the constraints placed on the design.

When mathematical optimisation techniques are applied to such problems it becomes inevitable that derivatives or sensitivities of the device response with respect to design variables are required in order to describe the objective and constraint functions. The solution of the equations governing device response is a time consuming and hence costly process and subsequently the calculation of design derivatives will form a major part of the total solution process.

This situation is further compounded due to the nonlinear behaviour of device response thus it becomes imperative that computationally efficient techniques are adopted in order that solution times can be kept within reasonable limits.

The purpose of this paper is to investigate the efficient calculation of design derivatives for nonlinear continuum problems and also to present a technique whereby these may be applied in the optimal design of semi-conductor devices. Sensitivity analysis is discussed in the context of nonlinear applications and a solution scheme for design derivative calculation is presented. Examples are given for the calculation of design derivatives for diffusivity problems (quasi-harmonic equations) and these are compared with known analytical solutions.

Finally it is proposed to use this method of modelling in the solution of device design and the possibility of its application in the optimal design of bevelled and etched p-n junctions are described.

2. OPTIMISATION CONCEPTS OF OFF-STATE SEMICONDUCTORS

Consider the two-dimensional Poisson's equation (1) which governs the potential distribution across a p-n junction under reverse-bias for off-state conditions

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} = - \frac{\rho(\psi, x, y)}{k_r \varepsilon_o} \tag{1}$$

Applying the finite element method to approximate the potential distribution across the device and adopting the Galerkin weighted residual approach [3] the equations can be written in matrix form as

$$[C]\{\psi\} = \{Q(\psi)\} \tag{2}$$

where [C] is the constant capacitance matrix (ψ) is the potential vector and $\{Q(\psi)\}$ is the highly nonlinear charge vector.

The correct termination of high-voltage power devices is such that it is imperative to obtain the lowest possible peak electric field ε_{max} at the device edge. For instance if the device termination is poorly designed that it is possible for breakdown voltages of less than 50% of the ideal abrupt parallel plane junction to occur. This would subsequently cause an

undesirable increase in the device on resistance by as much
as a factor of five. High voltage termination techniques are
reviewed by Baliga [4] and suggest that doping density distri-
bution and geometric configurations are the most important design
variables for which an optimal solution could be sought to mini-
mise the maximum electric field ε_{max}.

The optimisation problem can be stated in discretised form
as

$$
\begin{array}{l}
\text{Min } z(x_n) \cong \text{Min} \quad (\max_i \varepsilon) \\
\qquad\qquad\quad (x_n) \\
\text{subject to } g_r(x_n) \le 0
\end{array}
\tag{3}
$$

where x_n is the set of design variables, i is the discrete set
of sampling points and ε is the electric field. In such problems
the functions $z(x_n)$ and $g_r(x_n)$ are usually implicit functions
which are dependent on the nodal coordinates or element bound-
aries which are described by x_n. Many investigators [5][6]
seeking the solution to equation (3) have resorted to sequential
programming and furthermore have approximated the objective
and constraint functions by applying first order Taylor series
as follows

$$
z(x_n) \cong z(x_n^k) + \sum_{j=1}^{n} (x_j - x_j^k) \left(\frac{\partial z^k}{\partial x_j} (x_n) \right)
\tag{4}
$$

and similarly

$$
g_q(x_n) \cong g_q(x_n^k) + \sum_{j=1}^{n} (x_j - x_j^k) \left(\frac{\partial g^k}{\partial x_j} (x_n) \right), \quad q = 1, r
\tag{5}
$$

The unknown terms in these equations are the so-called
design sensitivities or design derivatives $\frac{\partial z}{\partial x}$ and $\frac{\partial g}{\partial x}$ and these
must be determined such that equations (4) and (5) can be des-
cribed explicitly.

If the finite element method is used in the analysis phase
it becomes mandatory that accurate and efficient techniques are
adopted for the calculation of these sensitivities otherwise
modelling of equations (4) and (5) can be both time consuming
and furthermore inaccurate. The calculation of design sensit-
ivities has generally been applied to systems which exhibit
only linear behaviour. If semi-conductor devices are to be
considered then the governing equations are nonlinear even for
simple off-state devices. Thus it is the purpose of this paper
to develop and test the process of calculating design sensit-
ivities such that accurate mathematical models can be generated
for systems which exhibit some form of nonlinearity.

3. SENSITIVITY DERIVATIVES IN NONLINEAR PROBLEMS

Consider firstly the usual stiffness formulation which
produces a system of equations

$$[C]\{\psi\} - \{Q\} = 0 \tag{6}$$

If equation (6) is linear then the sensitivities can be found by differentiating this expression and upon rearranging yields the well known force derivative form of

$$\left\{\frac{\partial\psi}{\partial x}\right\} = [C]^{-1} \left\{\frac{\partial Q}{\partial x} - \frac{\partial[C]}{\partial x}\{\psi\}\right\} \tag{7}$$

Computationally equation (7) is equivalent to solving equation (6) with multiple right hand sides which can be undertaken at a considerable saving over the usual n+1 analyses. This technique will now be extended for the treatment of nonlinear problems. Many nonlinear problems such as diffusion and electrostatics can be described by the quasi-harmonic equation

$$\frac{\partial}{\partial x} k_x \frac{\partial\psi}{\partial x} + \frac{\partial}{\partial y} k_y \frac{\partial\psi}{\partial y} + Q = 0 \tag{8}$$

Nonlinearities often arise in such equations due to the physical dependence of k_x and k_y on the unknowns ψ. Euqation (8) can be readily solved by the finite element method in which the nonlinear dependency $[C(\psi)]$ is treated by applying iterative techniques as described by Lyness et al [7]. Rewriting equation (8) in matrix form and assuming that $[C]$ is dependent ψ we have

$$[C(\psi)]\{\psi\} - \{Q\} = 0 \tag{9}$$

For some initialising value (ψ°) equation (9) is generally not satisfied and an iterative process is implemented. If this process is convergent then the equation is said to be satisfied when the error is less than some preassigned index e. If we consider that for some problem a solution has been found for some relatively small error e then equation (9) can be considered to be balanced or that the equality holds. This implies that we can operate on this equation in a similar manner to that of equation (7). Thus on differentiating equation (9) and re-arranging we have

$$\left(\frac{\partial\psi}{\partial x}\right) = [C(\psi_{p-1})]^{-1} \left[\frac{\partial Q}{\partial x} - \frac{\partial[C(\psi_{p-1})]}{\partial x}\{\phi_p\}\right] \tag{10}$$

where p denotes the number of iterations required to achieve convergence of the original set of equations to within some preassigned error index e.

On inspection of equation (10) it can be seen that some error has been introduced due to the iterative nature of the solution of the initial set of equations (9). In fact the stiffness terms $[C(\psi)]$ and $\frac{\partial[C(\psi)]}{\partial x}$ are evaluated at the p-1th iteration while the variable (ψ) is evaluated using the updated stiffness term $[C(\psi_p)]$ at the converged iteration p. This problem can however be dealt with by recalculating the stiffness and stiffness derivative terms using the converged values of

(ψ_p). This is equivalent to updating $[C(\psi)]$ in preparation for a further iteration of the nonlinear solution except here the requirement is to produce a more accurate solution to the right hand side of equation (10).

Thus equation (10) may be rewritten as

$$\left(\frac{\partial \psi}{\partial x}\right) = [K \ (\psi_p)]^{-1} \ \left(\frac{\partial Q}{\partial x} - \frac{\partial [K(\psi_p)]}{\partial x} \ \{\psi_p\}\right] \tag{11}$$

which can be considered to be the nonlinear form of equation (7).

The implementation of this system is described in figure 1 with the major changes being restricted to the frontal and stiffness routines. It should be noted that automatic redescription of the boundary geometry is required which allows perturbation of the design vector x_n. This is achieved by using a mesh generation system which calculates nodal coordinates as a function of the prescribed design variables.
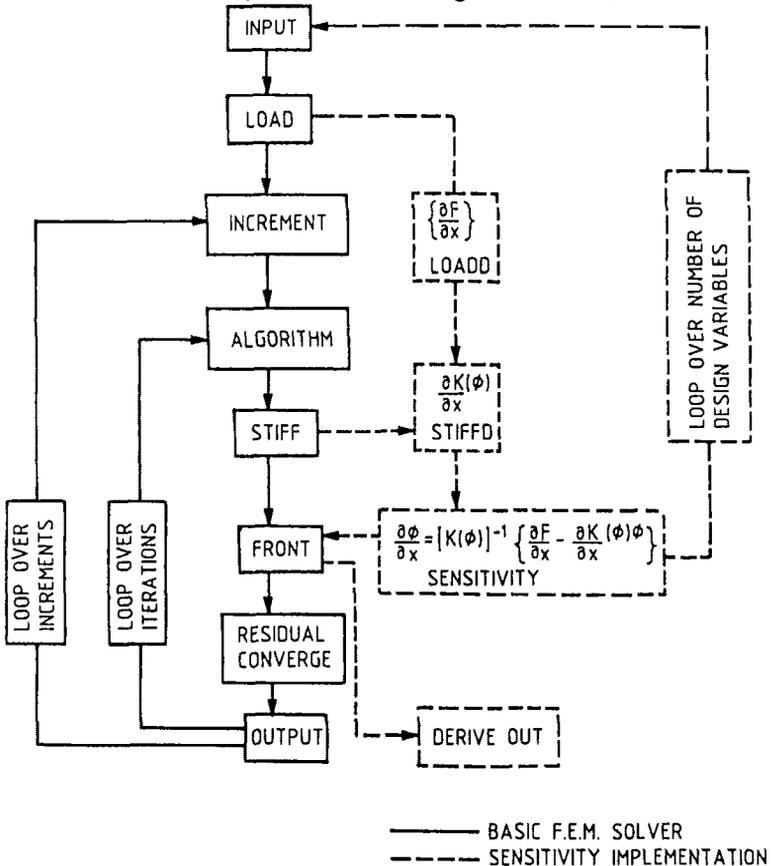

FIGURE 1 FLOW CHART OF NON-LINEAR F.E.M. PROGRAM
WITH MODIFICATIONS FOR SENSITIVITY ANALYSIS

4. APPLICATION TO A NONLINEAR PROBLEM

Consider a two dimensional problem of diffusion through a cylinder where some relationship exists between the diffusivity K and the concentration ϕ. The cylinder geometry and boundary conditions are shown in figure 2. The internal radius R_1 is the design variable of the system. We are interested in calculating the design derivatives $\partial\psi/\partial R_1$ which will define explicitly the mathematical model by equations (1) and (2).

In this example for simplicity a linear function relating diffusivity and concentration will be considered where

$$k_x = k_y = k_o (1 + \alpha\psi) \tag{12}$$

α is a coefficient with values $\alpha \geq -1$. The Q term of equation (8) is zero.

The analytical solution for this problem is presented in the text by Crank [8] and will be used for direct comparison with the numerical solution.

5. EXAMPLES

The thick cylinder domain was radially discretised into 10 eight-noded, parabolic, isoparametric elements, figure 2. The perturbation step of the inner boundary was $\Delta R = 0.005$ for all examples. Only the inner boundary nodes of the mesh were perturbated. The value of α was varied for the five examples shown so that the accuracy of the sensitivities could be compared for various strengths of nonlinearity and shapes of the ϕ distribution. The values of α chosen were $\alpha = 0$ (linear case), 0.5, 100, -0.5, -0.75.

The ϕ distribution for each value of α is plotted in figure 3. The finite element solution for the ϕ distribution showed excellent agreement with the analytical values.

The sensitivities $\partial\phi/\partial R_1$ calculated by the force derivative technique for each value of α have been tabulated in Table 1 to 3. The differenced analytical sensitivities are given together with the relative errors. The most erroneous results which are values of $\alpha = -0.5$ and -0.75 respectively are shown plotted in figures 4 and 5. Plots of $\partial\phi/\partial R_1$ from tables 1 to 3 have not been shown since the results are very nearly coincident.

It will be noticed that as $\alpha \rightarrow -1$ the gradient of ϕ near to the inner boundary increases appreciably. Correspondingly the error in the sensitivities increases. The problem dependency of this technique is thus apparent. However, for values of $\alpha \geq -0.5$, good agreement between the analytical and force derivative sensitivities can be shown and hence demonstrates the

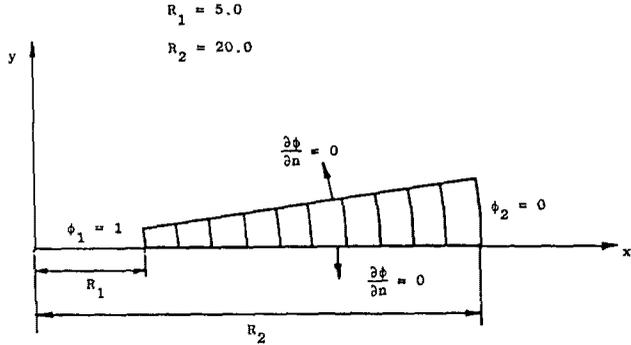feasibility of this method as applied to nonlinear continuum problems.

R$_1$ = 5.0

R$_2$ = 20.0

ϕ_1 = 1

$\frac{\partial \phi}{\partial n}$ = 0

ϕ_2 = 0

$\frac{\partial \phi}{\partial n}$ = 0

Fig. 2   10 element mesh for diffusion through thick cylinder

RADIUS	ANALYTICAL $\frac{\partial \phi}{\partial R_1}$	NUMERICAL $\frac{\partial \phi}{\partial R_1}$	RELATIVE ERROR
5.005	0.0	0.0	0.0
5.75	0.1297534	0.1299473	-0.0001938
6.50	0.1169916	0.1178129	-0.0008214
8.00	0.0953781	0.0959705	-0.0005924
9.50	0.0774899	0.0779913	-0.0005014
11.00	0.0622297	0.0626276	-0.0003978
12.50	0.0489234	0.0492372	-0.0003138
14.00	0.0371268	0.0373648	-0.0002379
15.50	0.0265321	0.0267022	-0.0001701
17.00	0.0169168	0.0170252	-0.0001084
18.50	0.0081151	0.0081671	-0.0000520
20.00	0.0	0.0	0.0

TABLE 1   Design Sensitivities for α = 0.0

RADIUS	ANALYTICAL $\frac{\partial \phi}{\partial R_1}$	NUMERICAL $\frac{\partial \phi}{\partial R_1}$	RELATIVE ERROR
5.005	0.0	0.0	0.0
5.75	0.1112788	0.1116732	-0.0003944
6.50	0.1030521	0.1025151	0.0005370
8.00	0.0882162	0.0859084	0.0023078
9.50	0.0749209	0.0715988	0.0033221
11.00	0.0626979	0.0588333	0.0038646
12.50	0.0512483	0.0472530	0.0039953
14.00	0.0403671	0.0365866	0.0037805
15.50	0.0299050	0.0266498	0.0032552
17.00	0.0197481	0.0173054	0.0024427
18.50	0.0098050	0.0084493	0.0013558
20.00	0.0	0.0	0.0

TABLE 2   Design Sensitivities for α = 0.5

RADIUS	ANALYTICAL $\frac{\partial \phi}{\partial R_1}$	NUMERICAL $\frac{\partial \phi}{\partial R_1}$	RELATIVE ERROR
5.005	0.0	0.0	0.0
5.75	0.0690817	0.0708727	-0.0017910
6.50	0.0655961	0.0672198	-0.0016236
8.00	0.0592269	0.0592269	-0.001347
9.50	0.0533839	0.0545398	-0.0011559
11.00	0.0478384	0.0487955	-0.0008620
12.50	0.0424153	0.0431826	-0.0007673
14.00	0.0369478	0.0375230	-0.0005753
15.50	0.0312318	0.0316073	-0.0003754
17.00	0.0249348	0.0250914	-0.0001566
18.50	0.0172622	0.0171563	0.0001059
20.00	0.0	0.0	0.0

TABLE 3   Design Sensitivities for $\alpha = 100$
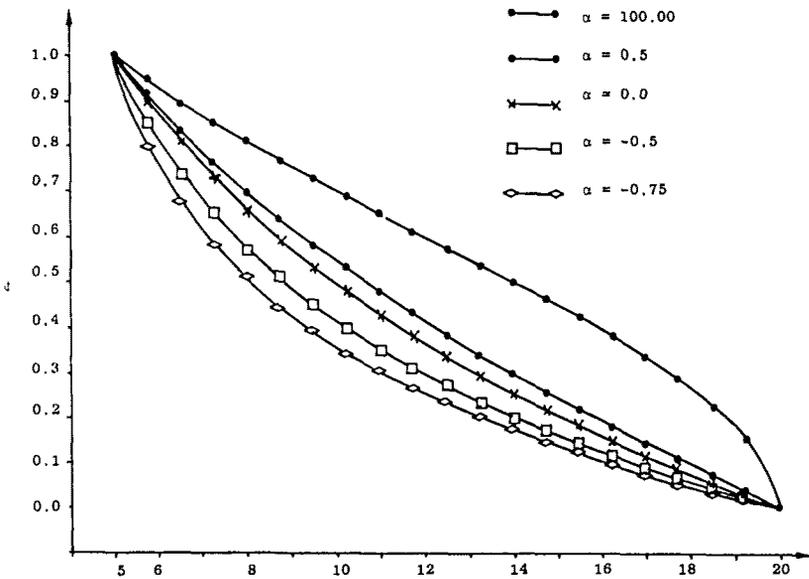
Fig. 3   Potential ϕ v Radius for various α values
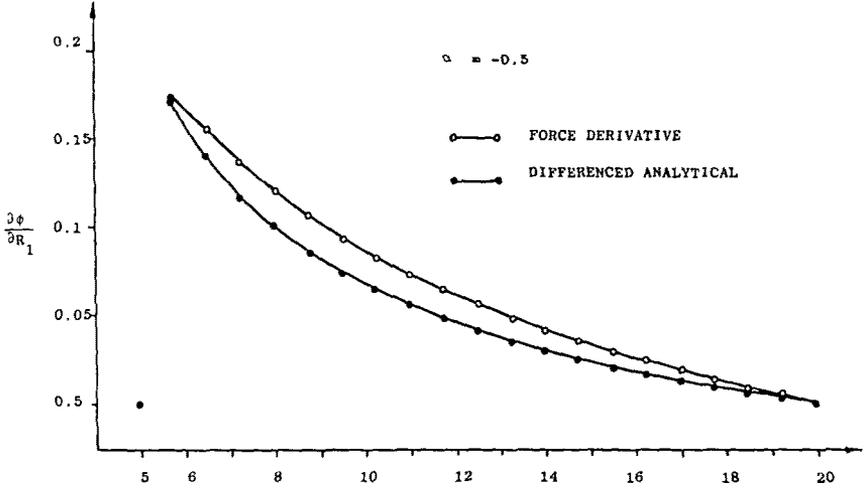
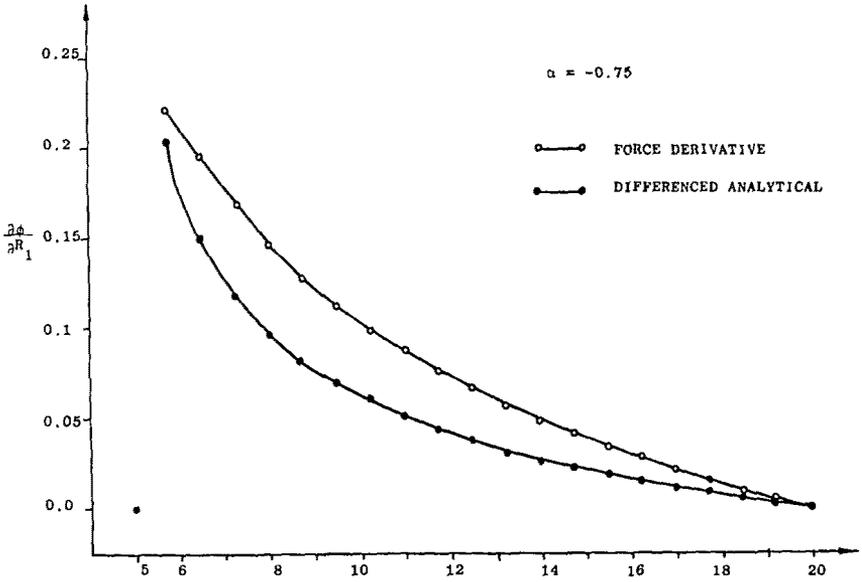Fig. 4   Design Sensitivity $\frac{\partial \phi}{\partial R_1}$ v Radius R, = -0.5

Fig. 5   Design Sensitivity $\frac{\partial \phi}{\partial R_1}$ v Radius R for α = -0.75

6. PROPOSED OPTIMAL DESIGN OF SEMICONDUCTOR DEVICES

From the previous section it has been shown that design sensitivites can be calculated for nonlinear field problems. The application of the force derivative technique to optimise the performance of off-state semiconductor devices is obviously apparent.

Differentiating equation (2) with respect to a design variable x_v and rearranging we obtain the potential sensitivity

$$\frac{\partial}{\partial x_v} \psi_p = C^{-1} \left[\frac{\partial Q}{\partial x_v} (\psi_p) \quad \frac{\partial C}{\partial x_v} \psi_p\right] \tag{13}$$

An exact difference of the derivative of the second term $\frac{\partial C}{\partial x_v}$, will be obtained in this case as the capacitance matrix is not a function of ψ. The Q vector would similary be updated with the ψ values from the converged solution as if preparing for a further iteration.

Once the potential sensitivities have been found the electric field sensitivities $\partial\varepsilon/\partial x_v$ can also be calculated. The electric field may be expressed in terms of the potential as follows

$$\varepsilon = -\nabla\psi \tag{14}$$

In the finite element notation this can be expressed as

$$\varepsilon = -[B]\psi_p \tag{15}$$

where the B matrix is the cartesian shape function derivatives. Differentiating equation (15) with respect to x_n we obtain the electric field sensitivities $\partial\varepsilon/\partial x_v$

$$\frac{\partial\{\varepsilon\}}{\partial x_v} = -\left\{\frac{\partial[B]^T}{\partial x_v} \{\psi_p\} + \frac{\partial\{\psi_p\}}{\partial x_v} [B]\right\} \tag{16}$$

where the derivatives of the B matrix $\partial[B]^T/\partial x_v$ can be found as described in [10].

This mathematical model describes the behaviour of potential distribution of the device in terms of the system variables and the next obvious step is its inclusion in a sequential optimisation technique. It is suggested that the move limit method with nonlinear programming would be particularly versatile since this would allow control over the accuracy of solution and is also generally applicable to problems which exhibit nonlinear response.

This procedure can be immediately adapted for the optimum design of many off-state semi-conductor devices. For instance consider the bevelled p-n junction shown in fig. 6. Here the
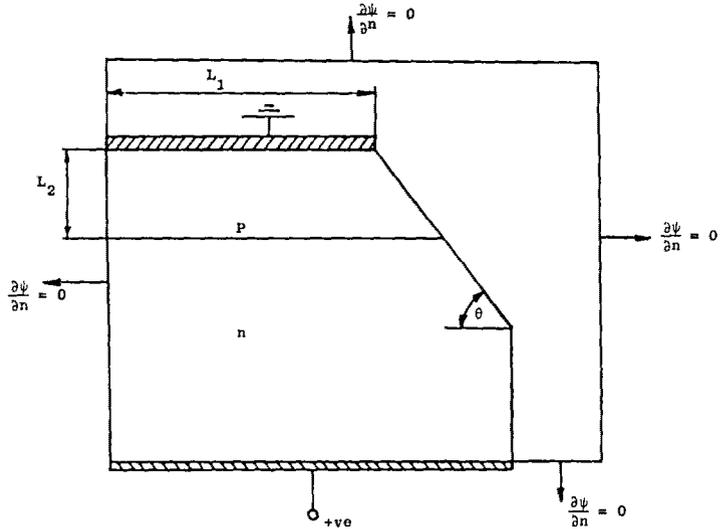
Fig. 6 Negative bevel, planar p-n junction

design variables are θ, L_1 and L_2 and relate to the device geometry. The optimum design would be the vector (θ, L_1, L_2) which minimises the maximum electric field within the device. Similarly consideration could be given to the important geometric configuration of etched p-n junctions. Here cubic splines could be utilised to define contour shpes thus enabling complex junctions to be developed whilst employing only a small number of design variables.

7. CONCLUSION

This paper demonstrates a feasible method for calculating design sensitivities for nonlinear field problems. The evaluation of these derivatives allows explicit development of the objective and constraint functions which may then be used to form the system model. An example of the technique applied to a diffusion problem gave good results and demonstrates that acccurate design derivatives can be obtained for nonlinear continuum problems.

Maximum utilisation of available software has been made with the main solver being based on well proven finite element programs. It is apparent that the implementation of sensitivity analysis in such situations only consumes a small fraction of the total computational time involved, the major portion being attributed to the solution of the nonlinear equations.

The extension of this technique to semiconductor devices is discussed and the related equations are derived for the calculation of design sensitivities.

The method is related to the optimum design of bevelled and etched p-n junctions and possibly geometrical layouts are proposed. It is envisaged that a fully sequential optimisation process based on design sensitivities could be highly beneficial in solving and redesigning the many device problems encountered in practice.

8. REFERENCES

1. BARNES, J. J., LOMAX, R. J.
    Finite Element Methods in Semiconductor Device Simulation.
    IEEE Transactions of Electron Devices, Vol.ED-24, No.8,
    August 1977.

2. ENGL, W. L., HEINZ, K. D. and MEINERZHAGEN, B.
    Device Modelling. Proceedings of IEEE, Vol.71, No.1, Jan-
    uary 1983.

3. ZIENKIEWICZ, O. C.
    The Finite Element Method, 3rd edition, McGraw-Hill Book
    Co. Ltd., 1977.

4. JAYANT BALIGA, B.
    High-voltage device termination techniques. A comparative
    review. IEE Proc. Vol.129, Pt.I, No.5, October 1982.

5. KIRSCH, U.
    Optimum Structural Design: Concepts, Methods and Appli-
    cations. McGraw-Hill, 1981.

6. FOX, R. L.
    Optimization Methods in Engineering Design. Addison-Wesley
    Publ. Co. 1971.

7. LYNESS, J. F., OWEN, D. R. J. and ZIENKIEWICZ, O. C.
    The Finite Element Analysis of Engineering Systems governed
    by a Nonlinear Quasi-Harmonic Equation. Computers & Struc.
    Vol.5, 65-79, 1975.

8. CRANK, J.
    The Mathematics of Diffusion. Oxford University Press,
    1967.

9. HINTON, E., OWEN, D. R. J.
    Finite Element Programming. Academic Press 1977.

10. FRANCAVILLA, A., RAMAKRISHNAN, C. V., ZIENKIEWICZ, O. C.
    Optimisation of shape to minimise stress concentration.
    Jour. of Strain Analysis, Vol. 10, No.2, 1975.