BOUNDARY ELEMENT METHODS FOR THE SOLUTION OF THE SEMICONDUCTOR EQUATIONS

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1. Introduction

Boundary methods have been used for some time as an alternative technique in the solution of linear potential problems (1). Only the boundaries are involved in the initial calculation with a linear system and once the values on the boundaries are fully evaluated, the solution within the domain may be obtained at any point by direct calculation. The equations are easily implemented numerically, paying due attention to singularities, require less storage and can easily be applied to irregular shapes. The techniques are placed in context and treated formally in Brebbia and Walker (2). A useful introductory discussion of methods of dealing with non-linearities is also included.

It is of interest to note that all of the representations, finite difference, finite element and boundary element are considered to be basically similar. This quickly becomes apparent if an attempt is made to obtain solutions for a particular problem using each of the three methods. It is therefore unlikely that a significant improvement could be expected to arise directly from the particular method employed. Nevertheless it is still worth investigating the different methods to see to what extent a particular type of problem can be treated more effectively using one method rather than another. Important factors could include the ease with which a given geometry may be represented, the way in which parameters and boundary values are to be stored and how the solution method is to be implemented. This is particularly important for a coupled non-linear equation set such as occurs in the solution of the semiconductor equations.

Solution methods for two-dimensional semiconductor device structures have now reached a stage where useful results can be obtained for simple cases. While reliable finite-difference programs, such as MINIMOS, are still being widely used, much of the recent work has concentrated on the application of finite-element methods, the equations usually being solved separately and the non-linearities taken into account through continuation methods with iteration and inversion of the Jacobian matrices associated with some form of Newton's method. While overall convergence in general cannot be guaranteed, particularly when the starting values are remote from the solution, it can still be expected when voltages are small and the geometry simple. The size of the matrices to be inverted, especially if the Jacobian is involved, and the corresponding computing times needed for an acceptable solution require the use of the largest available machines. Cost then becomes an important factor and may limit practical applications. Extension of the same methods to three-dimensional problems would also be seen to be expensive and uneconomic. Moreover, an increasing number of industrial designers are becoming accustomed to using personal, yet powerful, work stations. This trend justifies a search for formulations and methodologies which may permit the development of acceptably-accurate programs running on small machines in a reasonable time.

2. Possible Techniques

Two techniques in this area are being considered in the Electrical and Electronic Engineering Department at Queens University Belfast. The first involves the use of successive over-relaxation with finite elements. The method is not particularly new when applied to linear systems but may have some value in the simultaneous solution of the coupled non-linear semiconductor edquations, especially when starting values cannot be estimated accurately. It has been demonstrated to work particularly well for initial estimates with finite differences and poor starting conditions. The second technique is based on boundary integration. It is clear that the sparsity of information normally required from within the domain no longer holds when there are strongly non-linear charge/potential relationships contained in the equation set. All nodes or elements within the region contribute to the solution. However it is possible that some computational economy might still be achieved through an iterative solution method which requires the

inversion of the matrix relating only those variables and their normal gradients which exist along the boundary. Computation of the coefficients of the matrix now, of course, involves the whole domain over which a finite-element mesh must be established. Approximations are possible and a look-up table may be used.

The method proceeds by obtaining a first estimate of the quasi-fermi levels and the potential distribution within the domain. Charge and recombination can then be calculated and the unknown boundary values found from the related equation sets. Updated potential distributions can then be obtained. As with the linear solution, the correct boundary values, once computed, are sufficient to determine the hole and electron quasi-fermi levels and the electrostatic potential at any point within the domain. In practice, the interaction between charge and potential over the region prevents an explicit solution being obtained and iteration is again required.

Initial investigations indicate that the above problems may be overcome and useful solutions obtained. A major factor is the linearity of the original equation set. If the equations were completely linear, the answer could be obtained directly without recourse to iteration. Strongly non-linear terms may affect stability or make convergence slow or simply prevent a solution being obtained. A useful formulation has been developed by Yamaguchi (3). These equations contain more linear terms than the conventional versions. The linear terms give rise to the matrix coefficients and the non-linear terms, for the moment assumed constant, appear on the right-hand side. The more linear the equations, the more can be incorporated into the coefficient matrix. With the conventional version of the equations, there is very little left among the linear terms to contribute to the left-hand side of the equation set and a solution would appear to be virtually impossible.

3. Solution Method

Once a first estimate of the boundary values and the normal gradients have been obtained they can, in turn, be assumed to be constant. It then becomes necessary to calculate the potential distributions within the domain. The method is to use the values of charge and recombination from the previous iteration. These are assumed to exist at the centres of the triangular elements. They become singular sources,

along with the boundary values, with analytic potential solutions associated with each. The resultant contributions to the nodal potentials can then be computed or, to save time, can be stored in a triangular look-up table with zero entries where the contribution is considered to be small. No singularity problems arise since no boundary values are calculated and the element nodes cannot coincide with the centres of the elements. Using standard finite-element procedures, the charge and recombination in each element can be updated. These in turn can now be assumed to be constant and used in the boundary-element solution of the associated Poisson-like equations. The procedure is then repeated.

So far segments of the program have been tested and it is anticipated that some early results will be available shortly.

REFERENCES

1. F.S.Acton, *Numerical Methods that Work,* Harper and Row, New York (1970), p.439.

2. C.A.Brebbia and S.Walker, *Boundary Element Techniques in Engineering,* Newnes-Butterworths (1980).

3. K.Yamaguchi, *A Time-Dependent and Two-Dimensional Numerical Model for Mosfet Device Operation,* Solid State Electronics, 26. 907-916 (1983).