A Novel Finite-Element Approach to Device Modelling

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To efficiently simulate semiconductor devices, one has to take into account that regions where a broad grid spacing is sufficient may alternate with regions where a fine mesh is mandatory /4/. An adaptive mesh-refinement process has been developed which generates two different kinds of elements (triangles and rectangles) thus enabling almost arbitray subdivision and expansion of grid spacings. This guarantees that only the minimum number of nodes is created.

Another very critical decision in the application of the finite element method is the design of the shape functions. Cleverly chosen they can minimize the expected discretization error, especially if they anticipate the solution. It has been shown that linear/bilinear functions cause unwanted oszillations of the numerical solution and have, therefore, to be rejected /l/. This line of thought led to the development of shape functions for the exponentials of the quasi-Fermi potentials which are bilinear in Bernoulli-like functions. In elements where the carrier concentrations vary exponentially the discretization error is zero. These functions degenerate into the ordinary bilinear shape-functions when the electric potential is constant and into very steep functions when the electric field is large. The influence of the electric field on the shape functions will be illustrated and discussed. The electric potential itself is, consistently, approximated with linear/bilinear functions throughout the device.

This concept of variable and varying shape functions leads to a set of highly nonlinear equations. As weighting functions the linear/bilinear shape functions of the electric potential are used. The residuum integration is carried out numerically and the resulting nonlinear equations are solved using a modified Newton method. The Jacobian matrix is approximated by numerical differentiation /2/. An element-wise bypassing method for the calculation of the entries in the Jacobian matrix has been used to minimize computer requirements and actually enhance throughput. The Newton iterations, necessary for the solution of the nonlinear system, are accelerated using a damping procedure /3/. Specific examples will be shown to demonstrate the flexibility and accuracy of the outlined procedure.

- /1/ Buturla E.M. et al

 "Finite-Element Analysis of Semiconductor Devices: The FIELDAY Program"

 IBM J.Res.Develop., vol. 25(1981), no. 4, pp. 218-231
- /2/ Curtis A.R. and Reid J.K.

 "The Choice of Step Lengths When Using Differences to Approximate Jacobian Matrices"

 J.Inst.Maths.Applics.,vol.13(1974),pp.121-126
- /3/ Bank R.E. and Rose D.J.

 "Parameter Selection for Newton-Like Methods Applicable to Nonlinear Partial Diferrential Equations"

 SIAM J.Numer.Anal., vol.17(1980), pp.806-822
- /4/ Babuska I. and Rheinboldt W.C.

 "Error Estimates for Adaptive Finite Element Computations"

 SIAM J.Numer.Anal.,vol.15(1978),no.4,pp.736-754