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A Robust Finite Element Vector Formulation of the Semiconductor Drift-Diffusion Equations Incorporating Anisotropic Transport Properties

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The majority of commercial and academic licence semiconductor CAD software employs the one dimensional Scharfetter Gummel technique to estimate carrier flow between pairs of adjacent nodes coupled with a control volume method to effect integration of the continuity equations. Although applied successfully to 2-D and trapezoidal 3-D codes the technique suffers from a number of drawbacks. Firstly vector current densities can only be obtained by a process of averaging of the 1-D currents. This necessarily creates a degree of ambiguity in the method of averaging applied and casts doubt upon the simulated accuracy of physical effects which require an explicit knowledge of the current vector magnitude and direction (e.g. impact ionisation, thermal source terms, hydrodynamic models). Secondly, implementation of the control volume method requires particular care with respect to element shape. In 2-D the well documented obtuse angle problem has been identified as a source of solution instability whilst for 3-D simulations, employing arbitrary tetrahedral meshes, the problem of selecting an appropriate control volume is yet more difficult. Finally, many semiconductors have transport properties which are significantly affected by the orientation of the crystal lattice relative to the direction of carrier flux. For example, 4H-SiC exhibits a 20% higher mobility in the direction of the principle crystal axis [1]. A method based on an assembly of one dimensional currents cannot hope to provide accurate vector current estimates for material characterised by an arbitrary mobility tensor. Anisotropic behaviour has been successfully incorporated into Monte-Carlo simulations [2] but the computational cost of this technique rules it out for many CAD applications. In this paper, a new finite element vector formulation of the drift-diffusion model, including anisotropic effects, is introduced. Stability criteria for the model are described and a methodology is presented for providing stable solutions for spatial discretisations that include both acute and obtuse triangles, including cases where there is a large stretching of the element.

Anisotropic effects are incorporated into the basic drift-diffusion equations by representing the mobilities with second rank tensors e.g.

$$\mathbf{J}_n = \sum_{i=x,y}\sum_{j=x,y} \mathbf{e}_i \mu_{1n_{ij}} \left[\nabla_j n + n\mathbf{E}_{n_j}\right] \tag{1}$$

where $\mathbf{e}_i$ is the unit vector along the i axis and $\mathbf{E}_{nj}$ is defined as

$$\mathbf{E}_{n_j} = -\left[\nabla_j \psi_1 + \mu_{1n_{ij}}^{-1} \mu_{2n_{ij}} \nabla_j \psi_2\right] \tag{2}$$

The values ψ_1, ψ_2, μ_{1n} and μ_{2n} account for the fact that not all of the phenomena incorporated into the model necessarily exhibit the same degree of anisotropicity. The finite element expression of (1) is derived by adopting assumptions in keeping with the methods of Scharfetter and Gummel [3] and Bürgler *et al* [4]. Within a particular element it is assumed that the divergence of the current density is zero, (i.e. $\int_\Omega \nabla \cdot \mathbf{J}_n d\Omega = 0$) and that the current can be expressed as

$$\mathbf{J}_n = \sum_{i=x,y}\sum_{j=x,y} \mathbf{e}_i \mu_{1n_{ij}} \left[\nabla_j \xi + \xi\mathbf{E}_{n_j}\right] \tag{3}$$

where ξ is some arbitrary variable. The potentials ψ_1, ψ_2 and the variable ξ are represented in terms of linear interpolation functions and nodal values while the mobility within the element is assumed to be constant. With these assumptions the general form of the carrier concentration at any point within the element is given by

$$n = \xi + A\exp(-\mathbf{E}_n \cdot \mathbf{r}) \tag{4}$$

where $\mathbf{r}$ is the position vector of the location where the concentration, n, is calculated. To determine the constant A the zero divergence criterion is applied to (3) along with the linear representation of ξ [4]. This gives a solution for A of the form:

$$A = \frac{\int_\Omega \sum_{k=1}^{N} \mu_{n1} \mathbf{E}_n \cdot \nabla\varphi_k n_k d\Omega}{\int_\Omega \sum_{k=1}^{N} \mu_{n1} \mathbf{E}_n \cdot \nabla\varphi_k \exp(-\mathbf{E}_n \cdot \mathbf{r}_k) d\Omega} \tag{5}$$

where N is the number of nodes associated with the element, φ_k is the interpolation function for node k and μ_{n1} is the tensorial form of the mobility. Using equations (3), (4) and (5) the current can be expressed as:

$$\mathbf{J}_n = \sum_{k=1}^{N} \sum_{i=x,y} \sum_{j=x,y} \mathbf{e}_i \mu_{1nij} \left[n_k - \frac{\int_\Omega \sum_{m=1}^{N} \mu_{n1} \mathbf{E}_n \cdot \nabla \varphi_m n_m d\Omega}{\int_\Omega \sum_{m=1}^{N} \mu_{n1} \mathbf{E}_n \cdot \nabla \varphi_m \exp(-\mathbf{E}_n \cdot \mathbf{r}_m) d\Omega} \exp(-\mathbf{E}_n \cdot \mathbf{r}_k) \right] \left[\nabla_j \varphi_k + \varphi_k \mathbf{E}_{nj} \right] \tag{6}$$

Inspection of (6) reveals it to consist of a direct FE translation of the (non-upwinded) current equation, represented by the n_k term of the square bracketed expression, and an upwinding term, represented by the second term of the bracketed expression. Implementation of (6) into a numerical code raises a number of issues. In particular, methods of evaluating the upwinding term for the cases of zero field ($\mathbf{E}_n \to 0$) and high field ($\mathbf{E}_n \to \infty$) must be established. For the zero field case, terms in both the numerator and denominator tend to zero. By expressing the effective field $\mathbf{E}_n$ as $\mathbf{E}_n = \delta\tilde{\mathbf{E}}_n$, where $\tilde{\mathbf{E}}$ is a unit vector, an appropriate series expansion for $\mathbf{J}_n$ may be obtained. For the case of high electric field, terms of the form $\exp(-\mathbf{E}_n \cdot \mathbf{r}_k)$ may lead to numerical overflow problems. However, by correctly choosing the node from which to evaluate the position vector terms it is possible to ensure that the arguments of the exponential terms are always negative.

The stability of the formulation for different element shapes and field directions is illustrated in figure 1. This shows contour plots of the upwinding term as a function of spatial position of the third node of a triangular element with respect to the longest edge of the element. The dimensions are normalised so that the longest edge is of unit length and the element is oriented so that the longest edge lies along x-axis. A field of unit strength is applied in both contour plots. Figure 1(a) shows the contours obtained with the field applied almost perpendicular to the longest edge while in figure 1(b) the applied field is almost parallel to the longest edge. Figure 1(a) illustrates that the formulation is always stable when the field is perpendicular to the longest edge, thus allowing the elements with large stretch ratios to be created. When the field is parallel to the longest edge (figure 1(b)) the stability of the formulation is strongly dependent upon the position of the third node (with respect to the longest edge). Whenever the third node is positioned close to the arc between the black and white regions in figure 1(b) the formulation becomes unstable due to a singularity occurring in the upwinding term. In spite of this, elements with large stretch ratios will still be stable provided right-angle (or near-right-angle) triangles are used. These results lead the way to a methodology for producing a robust and accurate solutions on a spatial discretisation using a non-uniform triangular mesh in which both acute and obtuse triangles, including highly stretched elements, are present. This methodology uses adaptive meshing of the structure with the use of an advancing front algorithm [5] in which criteria for guaranteed stability and accuracy (as determined by an error estimator of some sort) of the solution are incorporated to allow the creation of an mesh where the elements are preferentially oriented to coincide with the direction of the field.

References

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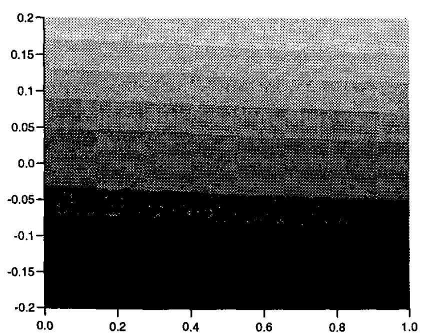
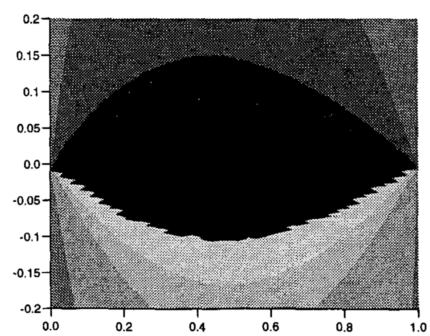


(a)



(b)

Figure 1. Contour plot showing upwinding term stability as a function of node position. (a) Field is almost perpendicular to longest element edge; (b) Field is almost parallel to longest element edge.