An New Discretization Scheme for the Semiconductor Continuity Equations

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ABSTRACT

We have developed a new, analytical hybrid finite element method to discretize the semiconductor continuity equations. Contrary to the popular box integration scheme of Scharfetter and Gummel, our technique is rather insensitive to the element geometry, thus avoiding the "obtuse" angle problems usually found in multi-dimensional simulations. Furthermore, a linear ansatz for the current in each element provides higher accuracy. The method works in any dimension and for (n-dimensional) simplexes as well as for quadrilaterals, bricks, prisms,etc. We have successfully tested it on various two- and three-dimensional problems.

Since the early days of numerical device simulation, the discretization of the semiconductor continuity equations has generated considerable interest in the modeling community. Starting with the one-dimensional case, the original work of Scharfetter and Gummel has been the commonly used method. Through the box integration scheme, it has been successfully extended to higher dimensions.

The shortcomings of the Scharfetter-Gummel Box scheme are well known. Their implications are the origin of considerable difficulties in the generation of "proper" grids and smooth solutions. While 2d grids can be optimized through user intervention, this is no longer possible for the simulation of complex 3d geometries. This justifies the need for a method that is almost independent of the geometrical shape of an element.

In the following, we derive the expression for a linear current j over an element. Starting from the expression for the current equation,

$$j = \mu_n e^{u} \nabla (e^{-v}) \qquad (1)$$

one can easily show that

$$\nabla \times j + E \times j = 0 \qquad (2)$$

where we used the electric field $E = -\nabla u$.

Remark: Equation (2) also shows the shortcoming of the multi-dimensional Scharfetter-Gummel scheme in that a constant current j would imply that either j is parallel to the electric field E, or the current j or the electric field E is zero. Neither of the two cases is true in general.

The most general current j satisfying Eq. (2) can be written as

$$j = \nabla \eta + \eta E = e^{u} \nabla (e^{-u} \eta). \qquad (3)$$

Using the definition for the current in Eq. (1), a constant mobility μ_n and Eq. (3), we get

$$\nabla \cdot (\mu_n e^{-v} - e^{-u} \eta) \equiv 0 \qquad (4)$$

or

$$\eta = \mu_n (e^{u-v} + \alpha e^{u}) = \mu_n (n + \alpha e^{u}) \qquad (5)$$

with the density n_i of electrons at point i.

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To determine α, we assume that inside a particular element

$$\nabla \cdot j = 0 \;, \tag{6}$$

We restrict ourselves to linear/bilinear currents such that η can be written in terms of linear/bilinear basis functions ϕ_i as

$$\eta = \sum_i \eta_i \, \phi_i \tag{7}$$

With Eq. (3) this leads to the condition

$$\nabla \eta \cdot E = 0 \,. \tag{8}$$

We write the function η in terms of the basis functions ϕ_k, put this into Eq. (8) and obtain

$$(n_i + \alpha \, e^{\psi_i}) \, E_i = (n_i + \alpha \, e^{\psi_i}) \int_T \nabla \phi_i \cdot E \; dV = 0 \tag{9}$$

Equation (8) completely determines α in Eq. (5). η is given by

$$\eta = \mu \sum_i \left(n_i - \frac{\sum_k n_k \, E_k}{\sum_k e^{\psi_{ki}} \, E_k} \right) \phi_i . \tag{10}$$

Using Eqs. (3) and (10), the current in each element is uniquely defined to be

$$j = \sum_i \mu \left(n_i - \frac{\sum_k n_k \, E_k}{\sum_k e^{\psi_{ki}} \, E_k} \right) (\nabla \phi_i + \phi_i \, E) \tag{11}$$

The element stiffness matrix is then assembled with standard nodal basis functions and exact numerical quadratures.

In terms of the element matrix, the above scheme resembles the more classical streamline diffusion methods proposed recently. Each scheme can be viewed as adding an artificial diffusion term to the original equation.

A typical example of the power of the new method is illustrated in the series of three plots below. A simple pn diode structure in reverse bias has been simulated on a automatically generated grid with a large percentage of obtuse triangles (Fig. 1). The bias and potential distribution have been chosen to create a worst case, rectangularly shaped electric field of strenght 10^4 in the space-charge layer. Figures 2 and 3 allow a comparison of the original box method with our scheme. The box method generated an overshoot in the solution, whereas the hybrid

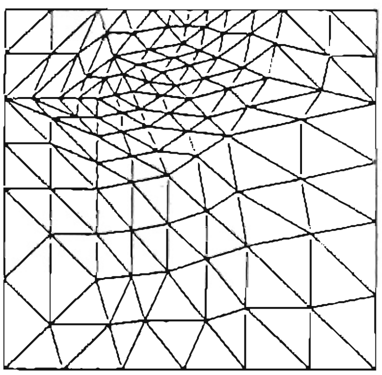

Fig. 1 Grid

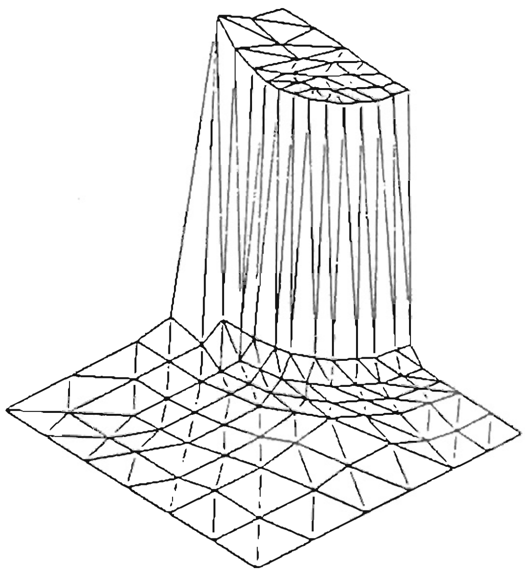

Fig. 2 Box Discretization

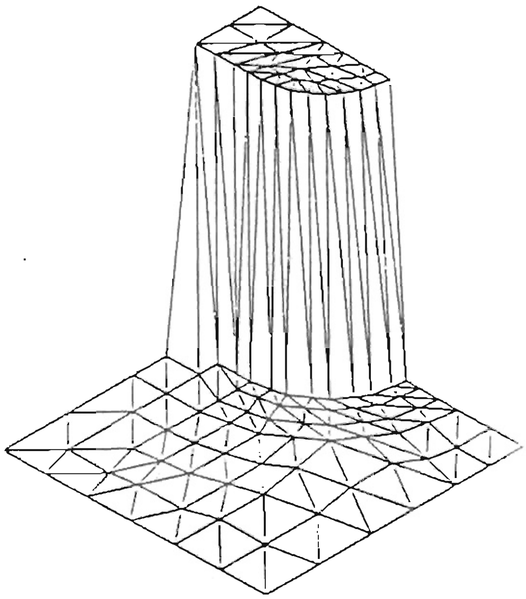

Fig. 3 New Discretization