Discretisation of the Hydrodynamic Transport equations using the Control Region Approximation

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Abstract *This paper focuses on the discretisation of the hydrodynamic transport equations for electrons in sub-micron MOSFET structures. In particular initialisation of the electron temperature equation, and the important problem of accurately calculating the energy input term ($\mathbf{J} \cdot \mathbf{E}$) on a generalised triangular FE mesh will be considered. The discretisation is applied to the calculation of substrate leakage currents in sub-micron LDD MOSFETs, the results of which will be presented.*

I. Introduction

As the size of active devices in VLSI sub-systems is continually reduced the validity of the standard drift-diffusion equations, as commonly applied to model semiconductor devices, is brought into question. The basic assumption made in the derivation of the drift-diffusion framework is that the charged carriers in a device are in thermal equilibrium with the lattice phonons at some ambient temperature.

The kinetic Boltzmann transport equation is the starting point for describing a many-particle carrier-phonon system, however, direct solution of this equation is a massive computational task and is therefore generally not attempted. A more practical approach is to use the first-five moments of the Boltzmann transport equation to provide an approximate solution which neglects the higher-order moments. These moment equations are commonly referred to as the hydrodynamic equations, which are basically conservation of charge, conservation of momentum (one in each of the three spatial dimensions) and the conservation of energy. This is an acceptable approximation provided there is sufficient randomisation of the thermal energy in the system to allow the meaningful use of average quantities such as velocity and effective carrier temperature. Under these conditions, the hydrodynamic equations, when used in the relaxation time limit, provide a practical engineering platform, which can be used to investigate hot-carrier effects such as velocity saturation and velocity overshoot.

This paper describes the discretisation of these equations using the Control Region Approximation. This method is general and is not restricted to a particular shape of element, however, we will assume the use of triangular elements. This has particular importance in the definition of the energy input into the energy moment equation. This will be discussed more fully in section 6.

II. Physical Equation System

Application of the moment method to the Boltzmann Transport Equation produces a series of equations, one for each moment taken. The resulting steady state electron energy moment equation can be written as

$$\nabla \cdot \mathbf{S}_n - \mathbf{E} \cdot \mathbf{J}_n + R w_n + n \frac{w_n - w_o}{\tau_{wn}} = 0 \tag{1}$$

here $\mathbf{S}_n$ is the energy flux vector, the second term describes the energy input into the system, and the last two terms describe energy loss in the system the first due to carriers recombining and the last due to inelastic collisions in the device. The average electron energy is described by w_n, R is the recombination rate and τ_{wn} is the energy relaxation time. The energy flux term is described by the constitutive relationship

$$\mathbf{S}_n = \mathbf{Q}_n - \frac{\mathbf{J}_n}{q}(w_n + kT_E) \tag{2}$$

here $\mathbf{Q}_n$ is a heat flux term which is identically zero under the symmetric Maxwellian assumption, however it is included heuristically here to account for the energy flow due to carrier thermal gradients.

The conservation of carriers is described by the steady state continuity equations for electrons and holes

$$\nabla \cdot \mathbf{J}_n - qR = 0 \tag{3}$$

$$\nabla \cdot \mathbf{J}_p + qR = 0 \tag{4}$$

which again require the constitutive relationships for flux in this case current densities. For electrons the appropriate moment equation along with the assumption that the momentum relaxation time is very short compare to the energy relaxation time leads to

$$\mathbf{J}_n = -q\mu_n n \nabla \psi + \mu_n k n \nabla T_E + \mu_n k T_E \nabla n \tag{5}$$

where μ_n is the electron mobility, n is the electron concentration, ψ is the electrostatic potential, k is the Boltzmann constant and T_E is the effective electron temperature. Hole transport is assumed to be described by the standard Drift-Diffusion framework.

$$\mathbf{J}_p = -q\mu_p p \nabla \psi + \mu_p k T_L \nabla p \tag{6}$$

where T_L is the ambient lattice temperature. Finally, Poisson's equation is solved for electrostatic potential

$$\nabla \cdot \mathbf{D} - \rho = 0 \tag{7}$$

where **D** is the electric flux vector given by

$$\mathbf{D} = \varepsilon \mathbf{E} = -\varepsilon \nabla \psi \tag{8}$$

ε is the dielectric constant for the material. Equations (1), (3), (4) and (7) along with the constitutive relationships (2), (5), (6) and (8) form a closed set of equations in the variables T_E, n, p and ψ. Which can be discretised using the control region approximation.

III Physical Models

Mobility model

At elevated electron temperatures carrier mobility is reduced by increased scattering rates this causes the carrier velocity to saturate. The electron temperature can now be used as a parameter in the electron mobility model. In effect it plays the same role as the electric field does in the standard drift-diffusion context. In this work an electron temperature dependent model is used which is consistent with the conventional field dependent model for mobility under homogeneous conditions, which has the form

$$\mu_n(T_E) = \mu_o \left\{ 1 + \lambda \left[\frac{k_B T_E}{q} - \frac{k_B T_L}{q} \right] \right\}^{-1} \tag{9}$$

μ_o is the low-field mobility and λ is related to the electron saturation velocity v_s and the energy relaxation time τ_{wn} by

$$\lambda = \frac{3}{2} \frac{\mu_o}{v_s^2 \tau_{wn}} \tag{10}$$

Impact Ionisation Model

In hydrodynamic simulations, non-local effects on carrier transport are of primary concern. Energy consideration in carrier transport plays a crucial role at this level of simulation. Accordingly, the suitability of using local field-dependent impact ionisation models in hydrodynamic simulations is not at all obvious. To alleviate this problem, the electric field dependence of the well-known Chynoweth's empirical formula for impact ionisation coefficient α_n is replaced by an appropriate electron temperature dependence. This requires the establishment of a relationship between the electric field and electron temperature. For the homogeneous case, the energy equation (1) together with the mobility model (9) can be used to obtain such a relationship

$$E = \left\{ \frac{3}{2} \frac{k(T_E - T_L)}{q \tau_{wn} \mu_o} \left[1 + \frac{\lambda k}{q} (T_E - T_L) \right] \right\}^{1/2} \tag{11}$$

Using the Chenoweth formula for α_n

$$\alpha_n = a \exp\left(-\frac{b}{|E|}\right) \tag{12}$$

where a and b are empirical coefficients, one can model the non-local effects of impact ionisation through the non-local solution of electron temperature.

IV Control Region Approximation

The partial differential equations that make up the device model are all in the divergence form, that is they have the divergence of some flux vector quantity and a number of source terms. In general then they can be written

$$\nabla \cdot \mathbf{F} - S(\mathbf{r}) = 0 \tag{13}$$

Over some local region of the device Ω performing a surface integral gives

$$\begin{aligned} &\iint_{\Omega} \nabla \cdot \mathbf{F} d\Omega - \iint_{\Omega} S(\mathbf{r}) d\Omega = 0 \\ &\Downarrow \\ &\oint_{\Gamma} \hat{n} \cdot \mathbf{F} d\Gamma - \iint_{\Omega} S(\mathbf{r}) d\Omega = 0 \end{aligned} \tag{14}$$

where $\hat{n}$ is the outward normal unit vector and Γ is the boundary of the region. This is now in a form suitable for discretisation. Consider a typical node i in a triangular mesh as shown in Figure 1.

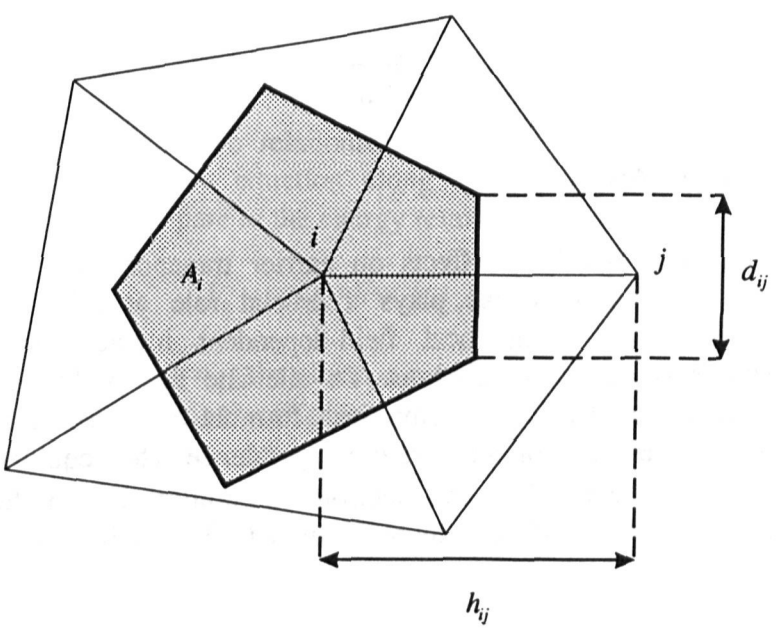

Figure 1. A control region Ω (shaded area), of area A_i, surrounding node i

The region of integration Ω becomes the Voronoi region (shaded) and the boundary Γ becomes the boundary of the Voronoi region. The line integral in (9) can now be approximated by a piece-

wise summation of the flux across each of the edge segments. The integration of the source term is approximated by assuming a it to be constant at the value found at the actual node, thus

$$\sum_{i=1}^{M_i} F_{ij} d_{ij} - S_i A_i \tag{15}$$

A_i is the Voronoi area associated with node i, M_i is the number of edge connected to the node, and d_{ij} is the pipe width connecting the nodes along line ij. So providing we can produce a suitable method of discretising the flux vectors along an edge we can apply (11) to all nodes in the mesh, the resulting set of non-linear equations can be solved using the Newton-Raphson method.

V Discretised form of the Semiconductor Equations

The set of divergence equations to solve are

$$\sum_{i=1}^{M_i} S_{nij} d_{ij} - \left(\mathbf{E} \cdot \mathbf{J}_n + R w_n + n \frac{w_n - w_o}{\tau_{wn}} \right)_i A_i = 0 \tag{16}$$

$$\sum_{i=1}^{M_i} J_{nij} d_{ij} - R_i A_i = 0 \tag{17}$$

$$\sum_{i=1}^{M_i} J_{pij} d_{ij} + R_i A_i = 0 \tag{18}$$

$$\sum_{i=1}^{M_i} D_{ij} d_{ij} - \rho_i A_i = 0 \tag{19}$$

The constituent relationships are readily discretised, for the first three equations the modified Scharfetter-Gummel method is used, and for the electric flux the standard finite-difference expression is used. The equations are assembled using the standard finite element approach on an element by element basis. The linear equations are solved using the Bi-CGSTAB method [1].

VI Discretisation of the Energy Source Term ($\mathbf{E} \cdot \mathbf{J}_n$)

This term provides energy input into the electron ensemble, and its proper discretisation is therefore essential. The difficulty in discretising this term arises from the inconsistencies of edge currents in a element. When the electric field ($\mathbf{E}$) is to be determined, a unique value for an element is readily found from the nodal potentials. This, however, this is not true for the current density field ($\mathbf{J}_n$), since the Scharfetter-Gummel method used in the discretisation will only yield consistent edge currents when the current flow is purely one-dimensional. In order to resolve this problem several techniques have been suggested [2,3,4]. The first method of Laux is found to be extremely unstable, especially in the drain depletion region, where there are rapid changes in carrier concentration and the weighting method can yield a distribution of heating which is both erratic and unrealistic. The other two methods use completely different approaches to the discretisation of the ($\mathbf{E} \cdot \mathbf{J}_n$) term, nevertheless, the discretised forms are almost identical apart from small second order differences. These terms have significant effect on the stability of the

solution procedure, since they occur in off diagonal terms of the system Jacobian, and under some conditions destroy the diagonal dominance of the system. This means that unless an extremely small mesh spacing is used, which is unphysical and computationally expensive, then a solution cannot be found for drain bias values over a few volts. For this reason the power scheme [3] is preferred, as it does not present any apparent convergence problems.

VII Solution algorithm

Figure 2 shows a flow diagram of the solution algorithm. Initially a fully coupled drift-diffusion solution is sought which is then used to provide an initial guess for electron temperature. It also provides a good guess for the other solution variables. A decoupled scheme is then used to obtain a self consistent solution of the hydrodynamic equations. Typically the number of iterations required for self-consistency increase with an increase in electron temperature.

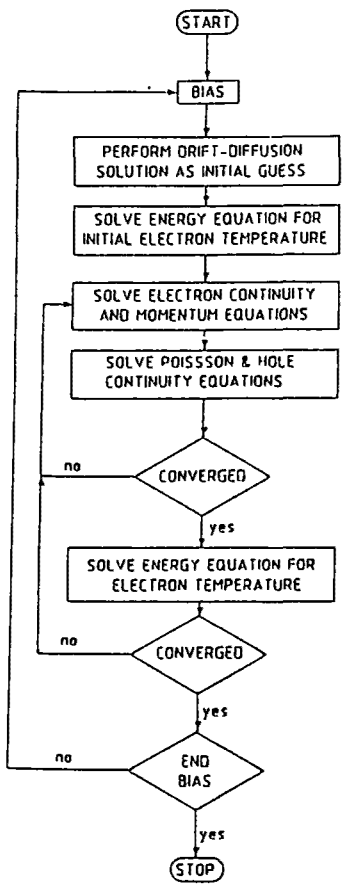

Figure 2. Algorithm for the solution of the hydrodynamic equations (16) - (19)

VIII Results

The results of the hydrodynamic simulation are demonstrated for a LDD device structure, and validated against experimental data on a range of devices of differing gate lengths. Figure 3 shows the electron concentration for a 5μm long channel device and the associated electron temperature. As expected the electron temperature is highest at the drain depletion edge, there is also a smaller amount of heating in the channel depletion region. Once the temperature distribution is established at a particular bias point the local impact ionisation rate can be calculated bas on the expression given in equations (11) and (12), from which the substrate current can be evaluated by summation across the device and weighting by the Voronoi area

$$I_{subs} = \sum_{\text{all nodes}} q n v_s \alpha_{ni} A_i \tag{20}$$

where v_s is the saturation velocity. Figure 4 shows the terminal currents for a 0.8μm length device, compared with experimental results for the same structure. In order to get such a good fit an energy relaxation time of 0.02ps has been used, and a saturation velocity of 9×10^6 cm/s has been used. The agreement with these same parameters is equally as good for shorter gate lengths.

IX Discussion

In his paper we have presented a self-consistent model capable of solving the hydrodynamic equations in semiconductor devices. The equations have been discretised on a general mesh using the control region approximation, careful consideration has been paid to the discretisation of the heat source term.

Results of the method have been demonstrated for an LDD MOSFET structure and found to give excellent agreement with measure drain and substrate currents.

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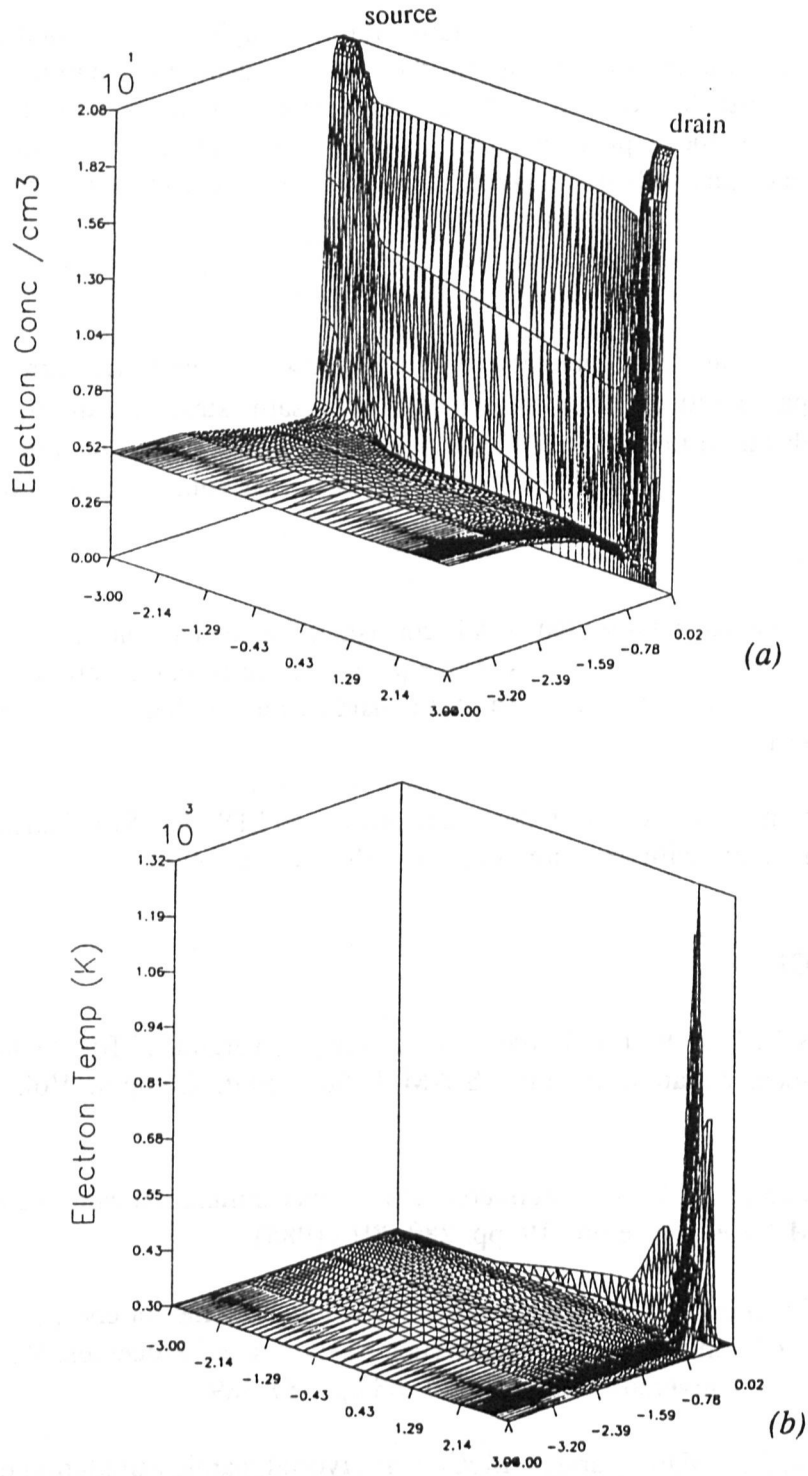

Figure 3. *(a) electron distribution VDS = 3.0V, VGS = 3.5 V*
(b) electron temperature VDS = 3.0V, VGS = 2.5V

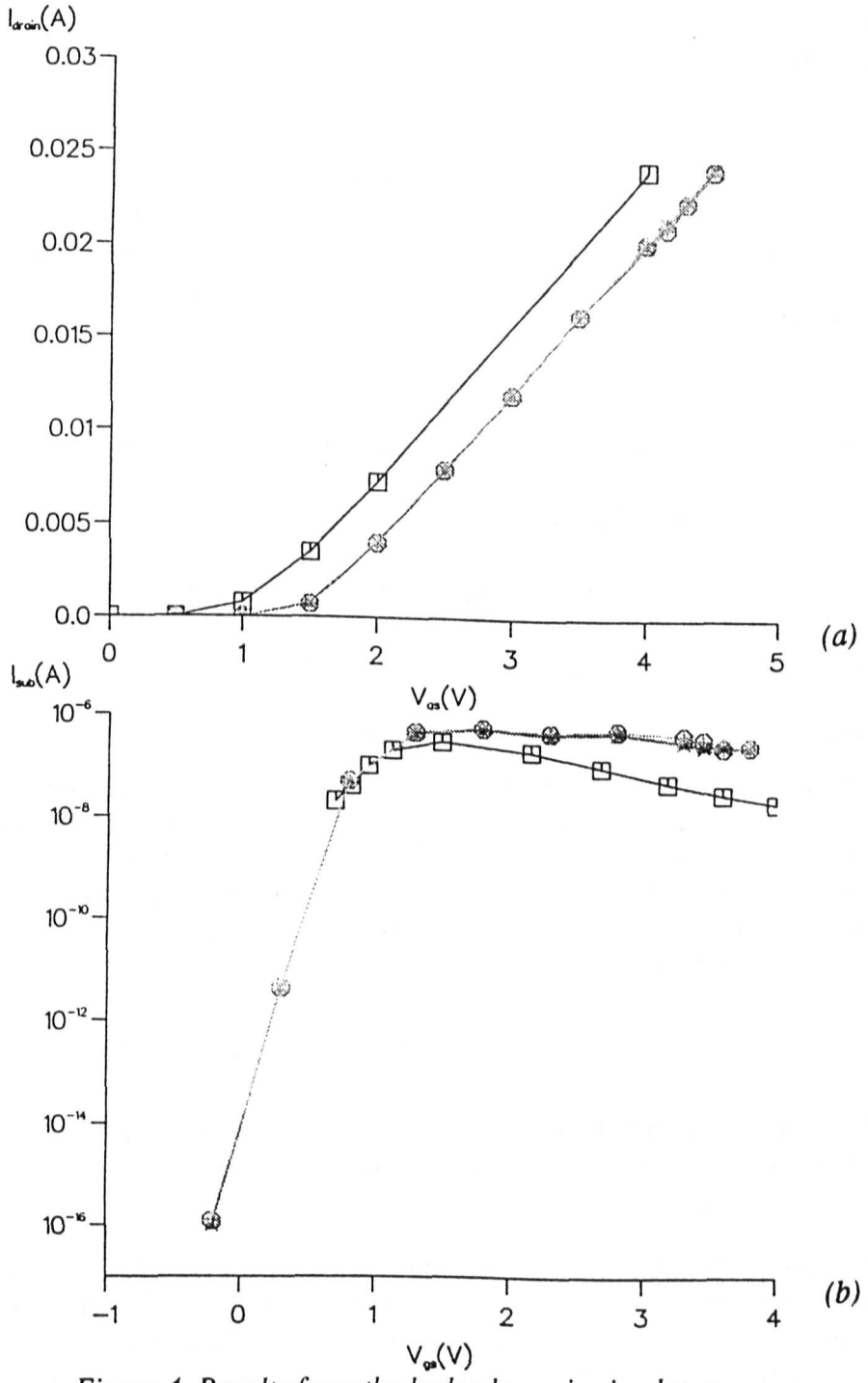

Figure 4. Results from the hydrodynamic simulator

(a) drain current - experimental (□) *and simulated* (O)
(b) substrate current - experimental (□) *and simulated* (O)