A Numerical Model of GaAs MESFET's Including Energy Balance for Microwave Applications

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Abstract—**Simulation of submicron semiconductor devices cannot be performed accurately using the drift-diffusion model (DDM), because of its inability to include nonlocal, hot carrier transport phenomena. Devices of these sizes require solution of the Poisson equation and the first three moments of the Boltzmann transport equation (BTE) [1]. These equations form a system of time-dependent, nonlinear, coupled, partial differential equations. The differential equations can be numerically solved using coupled or decoupled algorithms. Generally, coupled solvers require larger memory space and are computationally intensive, while conventional decoupled solvers have a limitation on the maximum time step which can be taken for transient solutions to less than the dielectric relaxation time (τ_d). A new decoupled solver has been developed that allows larger time steps than conventional decoupled Gummel algorithms and is less CPU memory and time intensive than coupled Newton solvers.**

I. Introduction

GaAs devices, such as MESFET's, are used at microwave frequencies, rather than Si devices, due to their higher gains and cutoff frequencies. In long channel GaAs MESFET's, the spatial variations of electric field and distribution function are generally gradual so that steady state is reached at every point in the device. This permits the two transport parameters, mobility and diffusion coefficient, to be considered to be local electric field dependent. In such cases, a modified version of the drift-diffusion model (DDM) can be used to simulate the devices.

In submicron devices, due to the rapid spatial variations of electric field and distribution function, mobility and diffusion coefficient can no longer be considered as dependent on the local electric field alone. The history of the carriers needs to be taken into account to determine carrier heating effects. It is, therefore, necessary to solve Boltzmann transport equation (BTE) and the Poisson equation, self-consistently, in these situations, to simulate the devices accurately. Monte Carlo or iterative methods can be used to solve the BTE and the Poisson equation. This is, however, computationally very expensive and has led to development of simpler models. Hydrodynamic transport equations are used to study nonstationary transport effects in submicron devices, as a compromise between speed and accuracy. These hydrodynamic transport equations are the first three moments of the BTE: the carrier continuity equation, the momentum balance equation and the energy balance equation. The momentum and energy relaxation times, carrier mobility and diffusion coefficients are energy-dependent parameters in these equations, and are obtained from Monte Carlo simulations of carrier transport in one-dimensional, uniform semiconductors at constant electric fields under steady state conditions. Further simplification of the momentum balance equation is possible, based on the fact that in most cases there is an order of magnitude difference in time scales between device and circuit time constants [2]. This results in a model called a quasi-hydrodynamic transport model, consisting of the simplified set of transport equations, also known as the balance equations, and the Poisson equation.

Manuscript received February 27, 1991.

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IEEE Log Number 9101080.

II. Transport Model

The quasi-hydrodynamic model consists of the following set of equations.

Poisson equation:

$$\nabla \cdot \epsilon \nabla \phi = -q(N_d - n). \tag{1}$$

Particle conservation equation:

$$\frac{\partial n}{\partial t} = -\nabla \cdot (nv). \tag{2}$$

Simplified momentum conservation equation:

$$nv = n\mu_e E + \mu_e \nabla (nkT_e). \tag{3}$$

Energy conservation equation:

$$\frac{\partial e}{\partial t} = qv \cdot E - \frac{\nabla \cdot (nkT_e v)}{n} - v \cdot \nabla e - \frac{(e - e_0)}{\tau_e(e)}. \tag{4}$$

where

ϕ	potential.
n	carrier concentration.
N_d	doping concentration.
v	carrier velocity.
E	electric field.
e	carrier energy.
μ_e	carrier mobility.
T_e	carrier temperature.
τ_e	energy relaxation time.

1051-8207/91/0700-0175$01.00

III. Numerical Method

Equations (1)–(4), form a set of nonlinear, coupled, time-dependent partial differential equations. These *differential* equations are discretized, using a finite-difference scheme over the solution domain to obtain nonlinear, coupled, time-dependent *difference* equations. These difference equations can be linearized and solved in a coupled manner (Newton method). The advantage of this method is that, theoretically, there is no constraint on the maximum allowable time step (Δt). But it should be noted that a very large "Δt" makes the initial guess of the solution to be very critical, and if very different from the true solution, can affect the overall convergence rate. This scheme, in general, requires larger memory space and is computationally intensive.

An alternative to this method is to solve the difference equations sequentially, in a decoupled fashion using a conventional Gummel algorithm. But, decoupling of the Poisson and carrier continuity equations introduces a restriction on the maximum allowable time step Δt, which needs to be kept smaller than the dielectric relaxation time of the material. The dielectric relaxation time is a function of doping and is approximately 10 fs for typical active layer concentrations, $N_d = 10^{17}$ cm^{-3}. Further, if the carrier continuity and energy balance equations are decoupled and solved sequentially, "Δt" must be kept less than the $\min(x^2/D_{\max})$ where x = grid spacing and $D_{\max}$ = maximum carrier diffusion coefficient [3]. Such limitations on the maximum time step Δt obviously require prohibitive computational resources for transient simulations, and especially for steady state problems.

Here, a new decoupled Gummel algorithm that allows Δt equal to as much as 10–20 $\times$ τ_d, is presented. In this scheme, the Poisson equation modified as shown next, and resulting equation is solved using a full implicit method

$$\nabla \cdot \epsilon \nabla \phi^{t+1} = -q\left(N_d - n^{t+1}\right) \tag{5}$$

at time level $(t + 1)$.

Rewriting n^{t+1} using Taylor series expansion, ignoring all $O(\Delta t^2)$ terms and substituting for $\left(\frac{\partial n}{\partial t}\right)_t$ from the continuity equation yields [4]

$$\nabla \cdot \epsilon \nabla \phi^{t+1} \cong -q\left(N_d - n^t + \Delta t \cdot \left(\nabla \cdot \left(-n^t \mu_e \nabla \phi^{t+1} + \nabla\left(D_e n^t\right)\right)\right)\right), \tag{6}$$

where D_e = carrier diffusion coefficient.

The potential, ϕ^{t+1}, is obtained by solving (6) using a full implicit method.

The continuity equation is approximated to first order accuracy in "Δt," $O(\Delta t)$, as

$$\frac{\left(n^{t+1} - n^t\right)}{\Delta t} = f\left(n^{t+1}, e^t\right), \tag{7}$$

where f is a function of n and e.

Therefore, the transport parameters, carrier mobility and the diffusion coefficient are lagged by one time step in the carrier continuity equation.

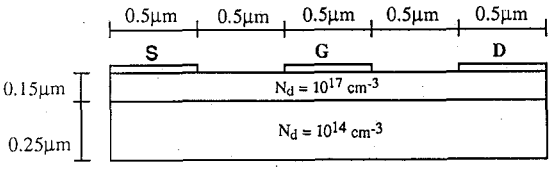

Fig. 1. GaAs MESFET structure used for simulation.

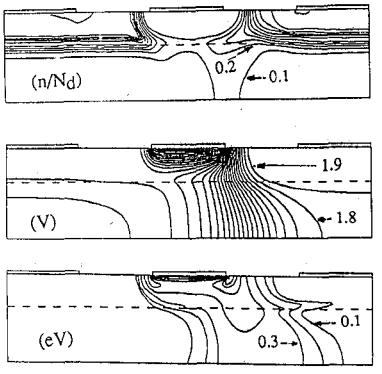

Fig. 2. Simulation results using conventional Gummel algorithm for the MESFET structure shown in Fig. 1, under bias conditions $V_d = 2.0$ V, $V_g = -0.5$ V at steady state. (a) Equi-concentration contour plot (normalized to N_d) in 0.1 N_d steps; (b) Equi-potential contour plot in 0.1 V steps; (c) Equi-energy contour plot in 0.1 eV steps.

Having obtained the potential and carrier concentration for the current time level to $O(\Delta t)$, the energy balance equation is solved for energy for time level $(t + 1)$. Since this equation is nonlinear, it must be first linearized and solved using the full implicit method. Since the Poisson and balance equations are solved to $O(\Delta t)$, independently of each other, the nonlinear iteration loop is eliminated in the new decoupled Gummel scheme.

IV. Results

The GaAs MESFET structure simulated is shown in Fig. 1. The structure consists of a 0.15 μm-thick active layer with doping concentration, $N_d = 10^{17}$ cm^{-3} on 0.25 μm-thick semiinsulating substrate ($N_d = 10^{14}$ cm^{-3}). The source/drain ohmic contacts are 0.5 μm-wide and 1.5 μm apart with a Schottky gate in between. For transient and steady state simulations of the terminal currents in this scheme, the time steps are gradually increased exponentially from "$\tau_d/2$" to "$10\tau_d$." The new Gummel scheme is found to be stable for time steps as large as 20 τ_d, in striking contrast to current conventional Gummel algorithms which do not converge for time steps, "Δt" $> \tau_d$. Figs. 2 and 3 show equi-carrier concentration, equi-potential and equi-energy contours at steady state obtained using a conventional decoupled and the new decoupled schemes respectively. The equi-carrier concentration contours are shown with the carrier concentration normalized to N_d. Table I shows the CPU times required to obtain steady state current values for the two different Gummel schemes, at different bias conditions, on a Cray Y-MP. There is a 5 – 7 X CPU time savings in the new Gummel scheme. Fig. 4 shows I_D–V_D characteristics of this GaAs MESFET structure, as evaluated by both schemes. It should be noted that the drain current does not saturate even at high $V_D > 3.0$ V. This is mainly due to

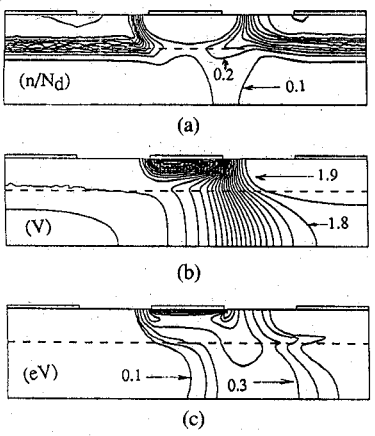

Fig. 3. Simulation results using new Gummel algorithm for the MESFET structure shown in Fig. 1, under bias conditions $V_d = 2.0$ V, $V_g = -0.5$ V at steady state. (a) Equi-concentration contour plot (normalized to N_d) in 0.1 N_d steps; (b) Equi-potential contour plot in 0.1 V steps; (c) Equi-energy contour plot in 0.1 eV steps.

TABLE I
CPU TIME TAKEN BY THE CONVENTIONAL GUMMEL ALGORITHM (OLD) AND THE NEW ALGORITHM ON A CRAY Y-MP TO OBTAIN STEADY STATE SOLUTIONS

Bias Conditions	Old Algorithm (CPU · s)	Old Algorithm I_D (mA)	New Algorithm (CPU · s)	New Algorithm I_D (mA)
$V_D = 2$ V, $V_G = -0.5$ V	860	88.7	142	88.0
$V_D = 4$ V, $V_G = -0.5$ V	910	99.6	151	101.1

carrier injection into the semi-insulating substrate. Carrier injection phenomena increases with the drain voltage, as can be seen by comparing the equi-carrier concentration contours shown in Fig. 3 and Fig. 5 for drain biases of 2.0 V and 4.0 V, respectively.

V. CONCLUSION

The order in which the quasi-hydrodynamic equations are solved exploits the large difference between the energy relaxation time, τ_e (typically 0.5 ps) and the dielectric relaxation time, τ_d (10 fs). Keeping the time step "Δt" smaller than the energy relaxation time τ_e gives better results because the relative change in energy in successive time steps is smaller than the relative change in carrier concentration. Hence the error introduced by using previous time level energies to obtain the transport parameters, μ_e and D_e, is smaller than if lagged values of carrier concentration were used in the energy balance equation.

A new decoupled scheme which is numerically stable for time steps Δt as large as $20 \times \tau_d$ is presented. This makes it possible to reduce Cray Y-MP CPU times by 5–7 X compared to those required by conventional Gummel algorithms, for steady state computations. This algorithm allows efficient analysis of GaAs MESFET's for microwave applications to study phenomena such as carrier heating near the drain, Gunn domain formation and carrier injection into the semi-insulating substrate.

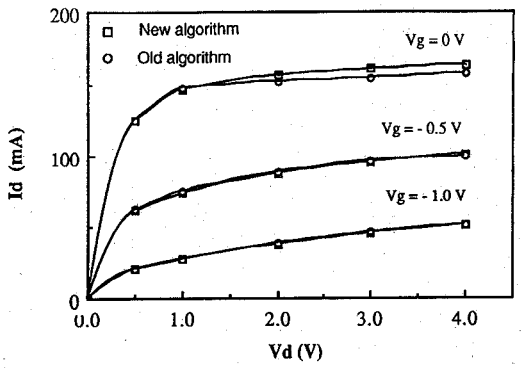

Fig. 4. Drain current (I_d) versus drain voltage (V_d) characteristics for the MESFET shown in Fig. 1.

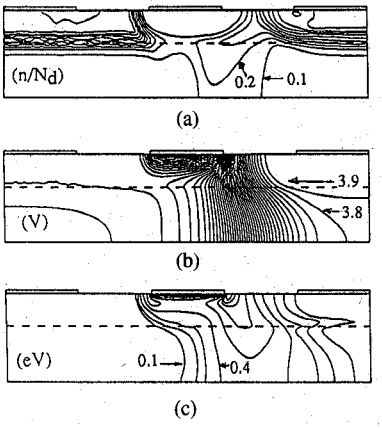

Fig. 5. Simulation results using new Gummel algorithm for the MESFET structure shown in Fig. 1, under bias conditions $V_d = 4.0$ V, $V_g = -0.5$ V at steady state. (a) Equi-concentration contour plot (normalized to N_d) in 0.1 N_d steps; (b) Equi-potential contour plot in 0.1 V steps; (c) Equi-energy contour plot in 0.1 eV steps.

REFERENCES

[1] Y.-K. Feng and A. Hintz, "Simulation of submicrometer GaAs MESFET's using a full dynamic transport model," *IEEE Trans. Electron Devices*, vol. 35, no. 9, Sept. 1988.

[2] C. M. Snowden, *Semiconductor Device Modeling*. London: Peregrinus, 1988.

[3] V. A. Nikolaeva, V. I. Ryzhii, and B. N. Chetverushkin, "Numerical simulation of nonequilibrium processes in an electron-hole plasma of binary heterostructures," *InzhenernoFizicheskii Zhurnal*, vol. 51, no. 3, Sept. 1986.

[4] ——, "A numerical method for the simulation of two-dimensional structures in the quasi-hydrodynamic approximation," *Sov. Phys. Dokl.*, vol. 33, no. 2, Feb. 1988.