ADI-FDTD Method for Physical Simulation of Semiconductor Devices

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Abstract—**This paper describes an alternating-direction implicit finite-difference time-domain method for the two-dimensional time-dependent simulation of semiconductor devices. This approach leads to the significant reduction of the semiconductor simulation time. We can reach over 80% reduction in the simulation time by using this technique while maintaining the same degree of accuracy achieved using the conventional approach. As the first step in the performance investigation, we use the electrons flow equations in the absence of holes and recombination in this paper.**

Keywords-ADI-FDTD Method; Semiconductor Devices; Drift-Diffusion Model; Physical Simulation

I. INTRODUCTION

Recently, a new method, called the alternating-direction implicit FDTD (ADI-FDTD) method, to solve Maxwell's curl equations has been introduced [1], [2]. This method is an attractive alternative to the standard FDTD due to its unconditional stability with moderate computational overhead. The unconditional stability means that the ADI-FDTD method is free of the Courant–Friedrich–Levy (CFL) stability restraint, allowing any choice of Δt for a stable solution. The ADI-FDTD can be particularly useful for problems involving devices with fine geometric features that are much smaller than the wavelengths of interest [3].

Many different approaches to the simulation of semiconductor devices have been developed in the past. All of these techniques are fundamentally dependent upon the solution of the Poisson equation along with the basic carrier transport equations. In this paper, the semiconductor analysis is based on the time-domain drift-diffusion method (DDM) [4]. The set of DDM equations contains the Poisson equation and the carrier transport equations, obtained by splitting the Boltzmann transport equation (BTE) into its first two moments. The DDM model assumes that the carrier temperature is equal to the semiconductor lattice temperature. Therefore, the carrier velocity is dependent on the electric field only. In comparison to other, more rigorous techniques for numerical modeling of semiconductor devices, the DDM is a relatively simple technique with better convergence of the algorithm and shorter computational times. Therefore, it is more suitable for use by a design engineer.

This paper presents a semi-implicit numerical method to solve the DDM equation based on ADI-FDTD scheme. This allows using a larger time-step size that leads significantly to CPU time reduction while maintaining the same degree of accuracy achieved using the conventional approach.

II. TRANSISTOR PHYSICAL MODEL

The semiconductor models used are based on the moments of Boltzmann's transport equations obtained by integration over the momentum space. Three equations need to be solved together with Poisson's equation in order to get the quasi-static characteristics of the transistor. This system of coupled highly nonlinear partial differential equations contains current continuity, energy conservation and momentum conservation equations [4]. The solution of this system of partial differential equations represents the complete hydrodynamic model. Simplified models are obtained neglecting some terms in momentum equation. One of these simplified models is drift-diffusion model (DDM). In this paper we simulate MESFET as microwave/mm transistor that is a unipolar device. For this device, the equations to be solved in the drift-diffusion model are

$$\nabla^2\phi = -\rho/\varepsilon = -q(N_d^+ - n)/(\varepsilon_0\varepsilon_r), \tag{1}$$

$$\frac{\partial n}{\partial t} = \frac{1}{q}\nabla\cdot\vec{J}_n = \frac{1}{q}\left(\frac{\partial J_x}{\partial x} + \frac{\partial J_y}{\partial y}\right), \tag{2}$$

$$\vec{J}_n = qn\mu_n(\vec{E}, N_d)\vec{E} + qD_n(\vec{E}, N_d)\nabla n, \tag{3}$$

$$\vec{E} = -\nabla\phi. \tag{4}$$

where $\mu_n = (\mu_0 + v_s E^3/E_s^4)/(1 + E^4/E_s^4)$ and $D_n = \mu_n K_B T/q$. In the above equations, ϕ is the potential, N_d^+ is the doping profile, n is the electron concentration, and μ_n and D_n are the mobility and the diffusion coefficient, respectively.

To have a numerically stable estimation of the electron concentration between nodes, we use the following equation [5]-[6] in directions x and y

$$n(c) = \{1 - g(c,\phi)\}n(a) + g(c,\phi)n(b)\ ;\quad c \in [a,b] \tag{5}$$

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where $g(c,\phi) = \{1\text{-}\exp(CV)\}/\{1\text{-}\exp(V)\}$, $V = (\phi_b\text{-}\phi_a)q/KT$, and $C = (c\text{-}a)/(b\text{-}a)$. Equation (1) can be discretized using the carrier concentration $n_{i,j}$ at $t = k\,\Delta t$ as the following

$$\frac{\phi_{i+1,j}-2\phi_{i,j}+\phi_{i-1,j}}{(\Delta x^2)}+\frac{\phi_{i,j+1}-2\phi_{i,j}+\phi_{i,j-1}}{(\Delta y^2)}=-\frac{q}{\varepsilon}(N_d^+-n_{i,j}^k). \quad (6)$$

By applying the ADI principle [6], the computation of (2) for the FDTD solution marching from the kth time-step to the $(k + 1)$th time-step is broken up into two computational sub-advancements: the advancement from the nth time-step to the $(k + 1/2)$th time-step and the advancement from the $(k + 1/2)$th time-step to the $(k + 1)$th time-step. More specifically, the two substeps are as follows.

Step 1) For the first half-step, i.e., at the $(k + 1/2)$th time step, the first partial derivative on the right-hand side (RHS) of (1), $\partial J_x/\partial x$, is replaced with an implicit difference approximation of its unknown pivotal values at the $(k + 1/2)$th time step, while the second partial derivatives on the RHS, $\partial J_y/\partial y$, is replaced with an explicit FD approximation in its known values at the previous nth time step. Using the first-order upwind scheme for spatial derivatives,

$$v_i\frac{d}{dx}[f_i]=\begin{cases}v_i(f_i-f_{i-1})/\Delta x & if\ \ v_i\ge 0,\\ v_i(f_{i+1}-f_i)/\Delta x & if\ \ v_i<0.\end{cases} \quad (7)$$

yields the following equation,

$$\begin{aligned}
&-\left[\frac{\Delta tD_{ij}}{2\Delta x^2}+\frac{\Delta t\,\mu_{ij}\alpha_{xi+1}(|E_x|+E_x)}{4\Delta x}\right]n_{i+1,j}^{k+1/2}\\
&+\left[1+\frac{\Delta tD_{ij}}{\Delta x^2}+\frac{\Delta t\,\mu_{ij}(\alpha_{xi+1}+\alpha_{xi})|E_x|}{4\Delta x}+\frac{\Delta t\,\mu_{ij}\nabla^2\phi}{2}\right]n_{i,j}^{k+1/2}\\
&-\left[\frac{\Delta t}{2\Delta x^2}D_{ij}+\frac{\Delta t\,\mu_{ij}\alpha_{xi}(|E_x|-E_x)}{4\Delta x}\right]n_{i-1,j}^{k+1/2}\\
&=\left[\frac{\Delta t}{2\Delta y^2}D_{ij}+\frac{\Delta t\,\mu_{ij}\alpha_{yj+1}(|E_y|+E_y)}{4\Delta y}\right]n_{i,j+1}^{k}\\
&+\left[1-\frac{\Delta t}{\Delta y^2}D_{ij}-\frac{\Delta t\,\mu_{ij}(\alpha_{yj+1}+\alpha_{yj})|E_y|}{4\Delta y}\right]n_{i,j}^{k}\\
&+\left[\frac{\Delta t}{2\Delta y^2}D_{ij}+\frac{\Delta t\,\alpha_{yj}(|E_y|-E_y)}{4\Delta y}\right]n_{i,j-1}^{k}.
\end{aligned} \quad (8)$$

where

$\alpha_{xi}=\dfrac{V_{xi}/2}{\Delta x\cdot Sinh(V_{xi}/2)}$ and $V_{xi}=\dfrac{\phi_{i,j}-\phi_{i-1,j}}{KT/q}$. The other value α_{yj} is calculated in similar manner in the y direction.

Step 2) For the second half time-step (i.e., at $(k + 1)$th time step), the second term on the RHS, $\partial J_y/\partial y$, is replaced with an implicit FD approximation of its unknown pivotal values at the $(k + 1)$th time step, while the first term is replaced with an explicit FD approximation in its known values at the previous $(k + 1/2)$th time-step. Using the first-order upwind scheme for spatial derivatives, the following equation cab be derived,

$$\begin{aligned}
&-\left[\frac{\Delta t}{2\Delta y^2}D_{ij}+\frac{\Delta t\,\mu_{ij}\alpha_{yj+1}(|E_y|+E_y)}{4\Delta y}\right]n_{i,j+1}^{k+1}\\
&+\left[1+\frac{\Delta t}{\Delta y^2}D_{ij}+\frac{\Delta t\,\mu_{ij}(\alpha_{yj+1}+\alpha_{yj})|E_y|}{4\Delta y}+\frac{\Delta t\,\mu_{ij}\nabla^2\phi}{2}\right]n_{i,j}^{k+1}\\
&-\left[\frac{\Delta t}{2\Delta y^2}D_{ij}+\frac{\Delta t\,\alpha_{yj}(|E_y|-E_y)}{4\Delta y}\right]n_{i,j-1}^{k+1}\\
&=\left[\frac{\Delta tD_{ij}}{2\Delta x^2}+\frac{\Delta t\,\mu_{ij}\alpha_{xi+1}(|E_x|+E_x)}{4\Delta x}\right]n_{i+1,j}^{k+1/2}\\
&+\left[1-\frac{\Delta tD_{ij}}{\Delta x^2}-\frac{\Delta t\,\mu_{ij}(\alpha_{xi+1}+\alpha_{xi})|E_x|}{4\Delta x}\right]n_{i,j}^{k+1/2}\\
&+\left[\frac{\Delta t}{2\Delta x^2}D_{ij}+\frac{\Delta t\,\mu_{ij}\alpha_{xi}(|E_x|-E_x)}{4\Delta x}\right]n_{i-1,j}^{k+1/2}.
\end{aligned} \quad (9)$$

Therefore the system of linear equations can be obtained which are symmetric and tridiagonal, and thus cheap to solve by methods like Choleski decomposition [8]. Fig. 1 shows flowchart of the sequence of ADI-FDTD scheme for DDF model.

III. Simulation Results

The transistor considered in this simulation is a 0.6 μm gate MESFET. Fig. 2 presents the conventional 2-D structure used for simulation. Here, a uniform mesh that covers the 2-D cross section of the MESFET is used (65×32).

The time-step size in the explicit methods for the semiconductor equations is a function of the average carrier velocity v_d and the spatial step to comply with the following CFL condition for stability and minimizing numerical dispersion [9],

$$v_d\Delta t\le\left[\frac{1}{\Delta x^2}+\frac{1}{\Delta y^2}\right]^{-1/2} \quad (10)$$

For the given cell size, the time-step sizes is about 10^{-15} s for conventional FDTD method. As the ADI-FDTD is unconditionally stable, a greater time-step size can be used for it. Here, Δt will be increased by a factor of 100.

The device is biased and the dc parameter distributions

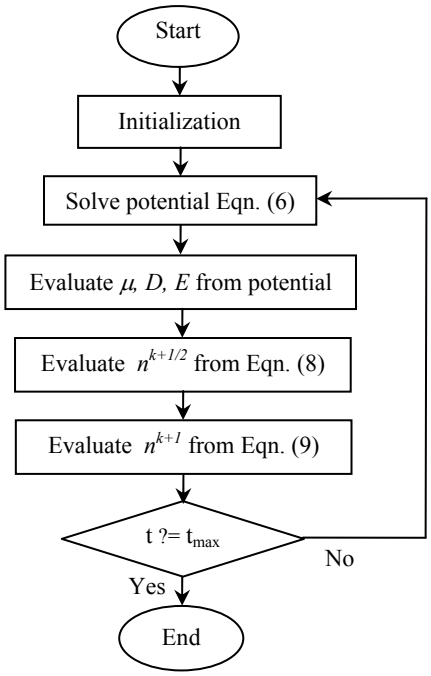

Figure 1. Flowchart of the sequence of ADI-FDTD scheme for DDF model.

(potential and carrier density) are obtained by solving the drift- diffusion model. The device is biased to V_{ds}= *2 V* and V_{gs}= *-0.5 V*. The state of the MESFET under dc steady state is represented by the distribution of potential and carrier density.

It is to be noted that Dirichlet boundary conditions are used at the electrodes while Neumann boundary conditions are used at the other walls.

Fig. 3 shows the potential and carrier density distributions obtained using the ADI-FDTD scheme. A comparison between results of different algorithms is provided in Figs. 4 and 5. It is significant to indicate that the ADI-FDTD method gives precisely the same results obtained when the FDTD method is used whereas in the case of using ADI-FDTD scheme, the CPU time is reduced by 83% with a maximum numerical dispersion error of 0.001%.

IV. Conclusion

This work proposed a numerical method for simulation of

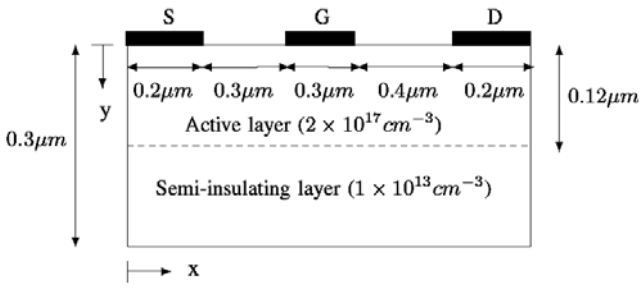

Figure 2. Cross section of the simulated MESFET.

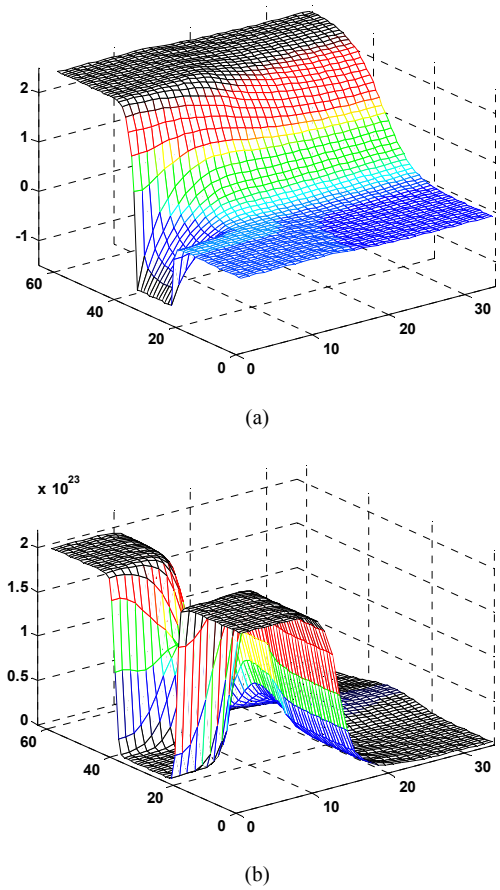

Figure 3. Sample DC results obtained using the proposed algorithm, (a) Potential distribution, (b) Carrier density distribution.

time dependent drift-diffusion model of semiconductor devices in two dimensions. Using the ADI-FDTD method to solve semiconductor equations allows increasing the time-step size by a factor of 100 and obtaining 83% reduction in the simulation time with a negligible error.

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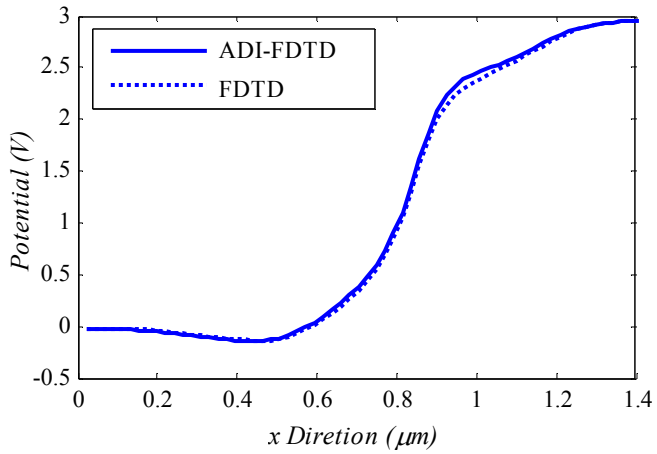

Figure 4. Potential distribution across the x direction for $y = 0.09$ μm.

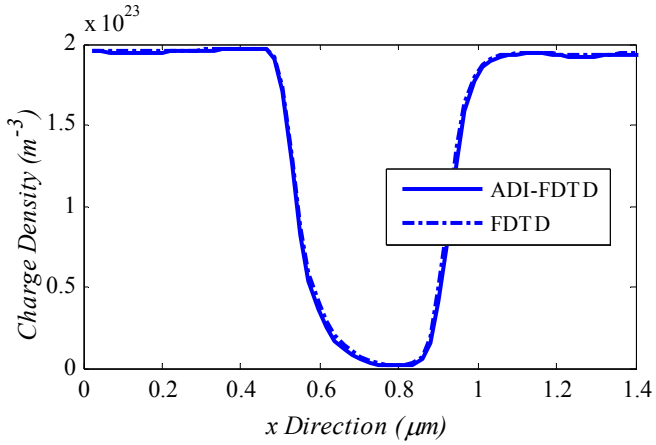

Figure 5. Charge Density (n) across the x direction for $y = 0.09$ μm.

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