IMPROVED SELF-CONSISTENT DEVICE MODELING BY DIRECT SOLUTION TO BOLTZMANN AND POISSON EQUATIONS

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Abstract

A new deterministic approach to device modeling where the the Boltzmann transport equation (BTE) and the Poisson equation are self-consistently solved has recently been reported[1]. With this new approach, the momentum distribution function for an entire device is efficiently calculated in approximately 1/100 the CPU time required of similar Monte Carlo simulations. While this new approach represented an advantage in computation times, achieving well-behaved numerical results has been difficult. To overcome these numerical difficulties, an improved numerical technique using a Scharfetter-Gummel-like discretization scheme and Slotboom-like variables has been developed. With this improved numerical approach, stable and nearly exponential convergence has been achieved. The output of this new technique is the space-dependent momentum distribution function (SDMDF) and the electric field for the entire device. Values of average electron energy and drift velocity calculated from the SDMDF agree well with Monte Carlo (MC) calculations, and require only a small fraction of the CPU time to evaluate.

1. The Model

The device model consists of the Poisson equation (1) and space-dependent BTE (2). These equations represent a coupled nonlinear system of partial differential-integral equations. The BTE incorporates the effects of a nonparabolic, multivalley, ellipsoidal band structure, as well acoustic, f-type and g-type intervalley phonon scattering and impact ionization. The transport model employed--deformation potentials, effective masses, etc.--is identical to the one used in popular Monte Carlo simulations[2]. Impact ionization is treated using a variation of the Keldysh approach[3,4]. The general form of the device model is given symbolically by:

$$\nabla_{\mathbf{r}}^2\phi(\mathbf{r}) = \frac{e}{\epsilon_s}\left[\frac{1}{4\pi^3}\int f(\mathbf{k},\mathbf{r})d\mathbf{k} - N(\mathbf{r})\right] \tag{1}$$

$$\frac{1}{\hbar}\nabla_{\mathbf{k}}\varepsilon \cdot \nabla_{\mathbf{r}} f(\mathbf{k},\mathbf{r}) + \frac{e}{\hbar}\nabla_{\mathbf{r}}\phi(\mathbf{r}) \cdot \nabla_{\mathbf{k}} f(\mathbf{k},\mathbf{r}) = \left[\frac{\partial f(\mathbf{k},\mathbf{r})}{\partial t}\right]_{ac} + \left[\frac{\partial f(\mathbf{k},\mathbf{r})}{\partial t}\right]_{iv} + \left[\frac{\partial f(\mathbf{k},\mathbf{r})}{\partial t}\right]_{ii} \tag{2}$$

where $\phi(\mathbf{r})$ is the potential; $N(\mathbf{r})$ is the doping concentration; $\mathbf{k}$ is the electron wave vector; ε is the electron energy; $\mathbf{r}$ is the electron position vector; $f(\mathbf{k},\mathbf{r})$ is the space-dependent momentum distribution function (SDMDF); the subscripts *ac*, *iv* and *ii* correspond to acoustic phonons, intervalley phonons and impact ionization respectively; and the integral of $f(\mathbf{k},\mathbf{r})$ in the Poisson equation provides the electron concentration.

To make the BTE tractable, we express the SDMDF in terms of Legendre polynomials:

$$f(\mathbf{k},\mathbf{r}) = f_0(\varepsilon,\mathbf{r}) + kf_1(\varepsilon,\mathbf{r})\cos\theta \tag{3}$$

where θ is the angle between $\nabla_{\mathbf{r}}\phi(\mathbf{r})$ and $\mathbf{k}$; $f_0(\varepsilon,\mathbf{r})$ and $kf_1(\varepsilon,\mathbf{r})\cos\theta$ represent the symmetric and the antisymmetric parts of the SDMDF respectively. By substituting the Legendre expansion into the BTE, it is transformed into a form which is complicated, but solvable numerically.

2. Method of Numerical Solution

With the BTE in a tractable form, we self-consistently solve the Poisson equation and BTE using a Gummel-type iteration scheme, along with a Scharfetter-Gummel-like discretization.

In our previous work, we used a direct, naive discretization. With this method, self-consistent solutions were achieved, however, convergence was slow, and limited to very low applied voltages[1]. Numerical problems were due to the exponential variation of the distribution function in both momentum and real space. Furthermore, the use of a naive discretization placed extra burden on the computer, requiring it to resolve the exponential variation of the distribution function. In the new discretization, the exponential resolution of the distribution function is performed analytically, thereby significantly reducing the computational requirements.

With the new improved method, we formulate a novel discretized expression of the BTE by using a Scharfetter-Gummel-like discretization scheme and Slotboom-like variables to resolve the exponential behavior of the distribution function. With this method the symmetrical part of the distribution function $f_0(\varepsilon, x)$ is expressed as the Slotboom-like form $f_0(\varepsilon, x)=n(x)q(\varepsilon, x)$; and the electron concentration $n(x)$ is given as $u(x)\exp\left(-\frac{\phi(x)}{V_t}\right)$, where $V_t = K_0T/e$. Here, we call $q(\varepsilon, x)$ the normalized distribution function. With the distribution function expressed in this form, the drift and diffusion parts of the BTE are formulated using a Scharfetter-Gummel-like discretization scheme. The result of this discretization yields a system which is extremely well-behaved numerically.

Once discretized, the system is solved using a Gummel-type iteration procedure. The BTE is solved using sparse matrices in the energy domain, and Gauss-Seidel iterations in real-space domain [1,5]. The 1-D nonlinear Poisson equation is solved using a globally convergent method [6].

To improve convergence of the Gummel scheme, we require that the current-continuity equation be satisfied explicitly, while accounting for the generation of excess carriers from impact ionization. Under these conditions, the 1-D continuity equation is written as

$$\frac{d\langle n(x)v(x)\rangle}{dx} = -\alpha_n(x)\langle n(x)v(x)\rangle \tag{4}$$

We have introduced $\alpha_n(x)$, which is the space-dependent ionization coefficient calculated from the SDMDF; and in our calculations, the expression for $\langle n(x)v(x)\rangle$ is written explicitly in terms of the symmetrical part of the distribution function, as shown in Ref. [5].

The explicit incorporation of the continuity equation facilitates convergence through the use of the Slotboom variable $u(x)$. This variable provides a weighting factor by which successive Gummel iterations are directed toward convergence. The weighting factor $u(x)$ is determined by solutions of the continuity equation. By combining values of the normalized distribution function $q(\varepsilon, x)$, the Slotboom weighting factor $u(x)$, and the potential $\phi(x)$, values for the distribution function are improved at each iteration step. Convergence is achieved exponentially, and the distribution function and electric potential are obtained self-consistently for the entire device. A flow chart of the calculation procedure is given in Fig. 1.

3. Results

We tested our new method on submicron devices with an $n^+ - n - n^+$ diode, which consists of $0.4\mu m$ n region with a constant doping concentration of $2 \times 10^{15} cm^{-3}$ sandwiched by two $0.1\mu m$ n^+ regions with doping concentrations of $5 \times 10^{17} cm^{-3}$. The ambient device temperature is $300°K$.

To demonstrate the success of the new discretization under high biases, in Figures 2 to 6 we show the results for an applied voltage of $5.0V$. In Fig. 2 the SDMDF, which has been multiplied by the density of states and divided by the electron concentration at each point, is plotted throughout the device. It is clear that in the left n^+ region, the field is low and thus the distribution function is similar to a Maxwellian; in the high-field n region, the distribution function is no longer Maxwellian and its peak spreads over a higher energy region to reflect the heating of the electron ensemble. Fig. 3 shows the values for electron concentration (dash line) and average velocity (solid line), and the agreement with MC simulations (open circles). Fig. 4 gives values of electric field (dash line), and average energy (solid line) which are in excellent agreement with the energy values calculated by MC methods (open circles). Fig. 5 shows the space-dependent impact ionization coefficients calculated by Eqn. (4) (solid line), ionization coefficients calculated directly from local values of the electric field (short dash line), along with the local-field (dot-long dash line). The figure shows that the peak and the falling edge of the impact ionization coefficients calculated from the space-dependent BTE are shifted to the right as compared to the field-dependent local model. This indicates the electrons remain fairly hot in the n^+ region for some distance, while the field-dependent local model neglects this nonlocal effect. Fig. 6 demonstrates the excellent convergence properties of the new discretization. In general, convergence is nearly exponential. Furthermore, when the applied bias is smaller, convergence is even faster. (The definitions of $|\Delta\phi|$ (solid line) and $|\Delta u/u|$ (dash line) in the figure are $|\Delta\phi| = \max_j \left|\phi_j^{k+1} - \phi_j^k\right|$, and $|\Delta u/u| = \max_j \left|(u_j^{k+1} - u_j^k)/u_j^{k+1}\right|$, respectively.) Another important advantage of the new discretization worth mentioning is that the number of nonuniform mesh points in real space was always chosen to be about 60, and is thereby essentially independent of applied bias.

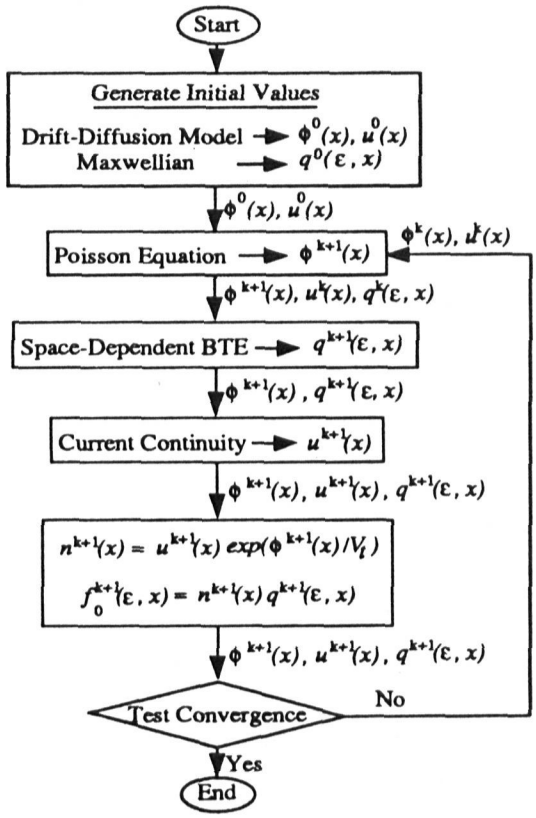

Fig. 1: The flow chart illustrates the device modeling procedures used in this work.

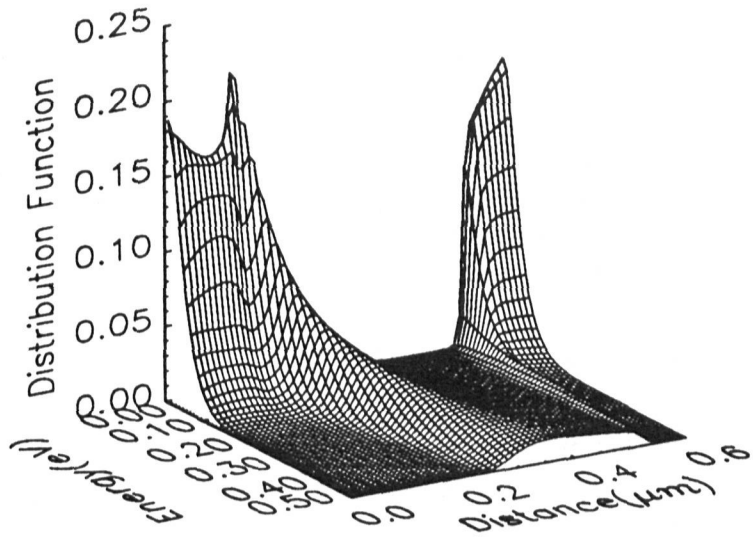

Fig. 2: Electron distribution function magnitude versus energy and distance

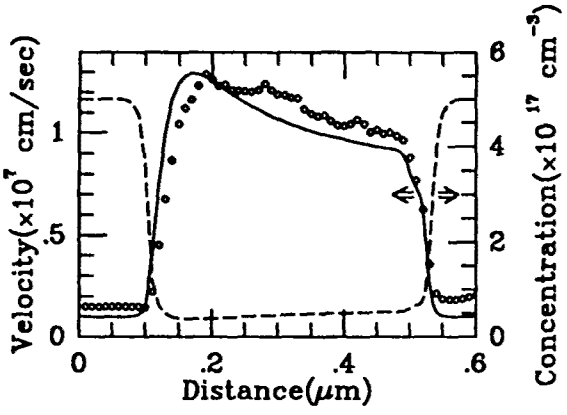

Fig. 3: Carrier concentration (dash line) and average velocity (solid line) calculated from this new method. Values for average velocity are shown to agree with MC calculations (open circles).

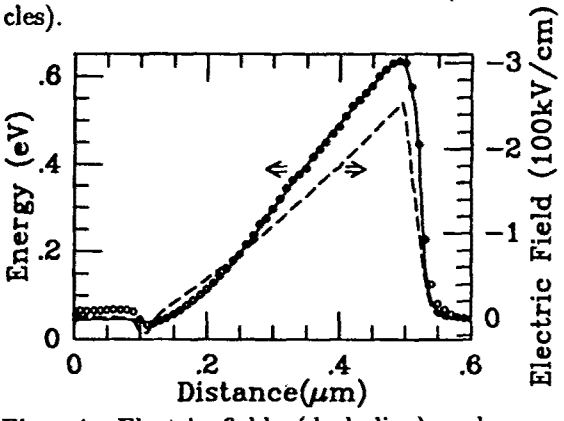

Fig. 4: Electric fields (dash line) and average energy (solid line) calculated from this new method. Values for average energy are shown to agree well with MC calculations (open circles).

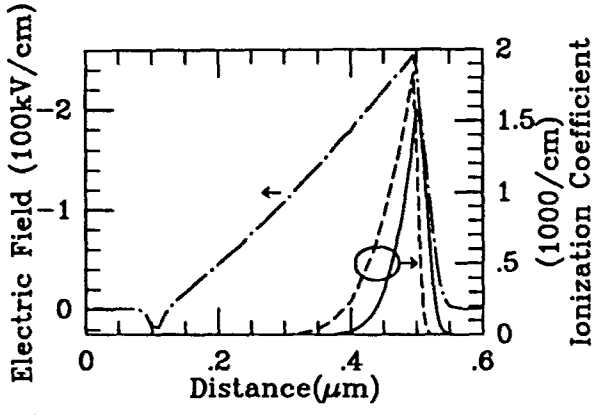

Fig. 5: Ionization coefficients calculated by this method (solid line) are compared with those obtained by the local field dependent method (dash line). Electric fields are plotted by a dot-long dash line for reference.

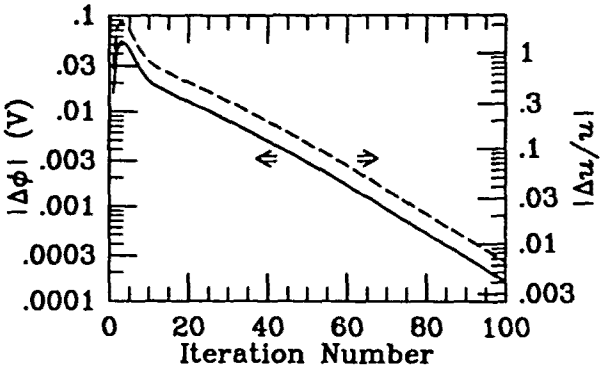

Fig. 6: The convergent rates for potential ϕ and Slotboom variable u are illustrated.

4. Conclusions

We have developed a new improved approach to device simulation by the direct, self-consistent solution to the Poisson and Boltzmann transport equations. With the method the BTE is formulated with a Legendre polynomial expansion. A new discretization of the Boltzmann equation has been developed using a Scharfetter-Gummel-like scheme and Slotboom-like variables to obtain a nearly exponential rate of convergence of the system. This new deterministic approach uses less than 1/100 the CPU time required by similar MC calculations. In summary, the new technique is promising for developing accurate simulators, which can be used for day-to-day efficient device modeling.

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References

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