Deterministic BJT Modeling by Self-Consistent Solution to the Boltzmann, Poisson and Hole-Continuity Equations

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Abstract

A new comprehensive and efficient bipolar junction transistor (BJT) device model is presented. This model self-consistently solves the Boltzmann transport equation (BTE) for electrons, the current-continuity equation for holes and the Poisson equation. The calculations provide almost the same information as similar Monte Carlo simulations, but require only 1% of the CPU time. In addition, a new discretization has been employed which facilitates convergence.

I. Introduction

In the past, device modeling by direct solution of the Boltzmann transport equation (BTE) was usually considered too difficult to be achieved. The difficulties were mainly due to dimensionality problems (the steady-state BTE is a 6-dimensional equation), and problems evaluating the complicated collision integral.

Recently, however, the Legendre polynomial (LP) technique has been demonstrated to provide fast and accurate solutions to the BTE[1,2,3]. Use of the LP technique allows one to overcome problems of dimensionality, and also facilitates evaluation of the collision integrals. However, until now the method was used only for very simple, largely unrealistic test structures[2], or only as a post-processor to hydrodynamic simulations[3]. Here, we overcome these limitations and adapt the new LP technique to actually model BJT's.

II. General Approach

In the present work we self-consistently solve the electron BTE, the Poisson, and hole-continuity equations to obtain the electron momentum distribution function for an entire prototype BJT. We first transform the BTE into a tractable expression using a first order LP expansion: this reduces the dimensionality of the system, and allows us to integrate the collision terms analytically.

To numerically solve the system, we first discretize the BTE using a new Scharfetter-Gummel-like algorithm which employs special state variables. After discretizing the Poisson and hole-continuity equations, the overall nonlinear system is then solved using a Gummel-type iteration scheme. This algorithm provides nearly exponential convergence to efficiently obtain the distribution function for the entire device without the statistical noise which is characteristic of Monte Carlo methods.

III. The Boltzmann-Poisson-Continuity System

The device model consists of the Poisson equation (1), the space-dependent BTE for electrons (2), and the current continuity-equation for holes (3). The collision integrals in the BTE account for the effects of acoustic and intervalley phonons, as well as impact ionization scattering. These scattering cross-sections, as well as nonparabolic conduction band-structure values, are identical to those employed in Monte Carlo calculations[4].

$$\nabla_{\mathbf{r}}^2\phi(\mathbf{r}) = \frac{e}{\epsilon_s}\left[n(\mathbf{r}) - p(\mathbf{r}) + N_A(\mathbf{r}) - N_D(\mathbf{r})\right] \tag{1}$$

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

$$\nabla_{\mathbf{r}}\cdot\left[\mu_p p(\mathbf{r})\nabla_{\mathbf{r}}\phi(\mathbf{r}) + \mu_p V_t \nabla_{\mathbf{r}} p(\mathbf{r})\right] = R(\phi, n, p) \tag{3}$$

where $n(\mathbf{r}) = \frac{1}{4\pi^3}\int f(\mathbf{k},\mathbf{r})d\mathbf{k}$ is the electron concentration; $p(\mathbf{r})$ is the hole concentration; $\phi(\mathbf{r})$ is the potential; $N_D(\mathbf{r})$ and $N_A(\mathbf{r})$ are the doping concentration for donors and acceptors; $f(\mathbf{k},\mathbf{r})$ is the distribution function; R is the recombination rate, including impact ionization and Shockley-Read-Hall (SRH) recombation; $V_t = K_B T/e$; the subscripts ac, iv, ii correspond to acoustic phonons, intervalley phonons, impact ionization, respectively.

IV. Method of Solution:

1. *BTE Formulation: Legendre Expansion*

We first express the distribution function in terms of Legendre polynomial basis functions:

$$f(\mathbf{k},\mathbf{r}) = f(\mathbf{k},x) = f_0(\varepsilon,x) + kg(\varepsilon,x)cos\theta \tag{4}$$

where θ is the angle between $\nabla_{\mathbf{r}}\phi(\mathbf{r})$ and $\mathbf{k}$; $f_0(\varepsilon,x)$ and $kg(\varepsilon,x)$ represent the coefficients of the symmetrical and the anti-symmetrical parts of the distribution function respectively.

In solving the BTE, our objective will be to determine the unknown coefficients f_0 and g. To determine these coefficients, we next substitute the Legendre expansion into the BTE, and use symmetry to obtain 2 equations for the 2 unknowns f_0 and g.

2. *Numerical Solution of BTE: A Scharfetter-Gummel-Like Approach*

At this point, the typical approach would be to discretize and try to solve the resulting equations directly. However, this direct approach would lead to a discrete matrix which is ill-conditioned, would not readily account for the exponential variation in the distribution function, and would inhibit obtaining a solution to the overall Boltzmann-Poisson-Continuity system.

To overcome numerical problems, and routinely solve the coupled system, we developed a Scharfetter-Gummel-like discretization scheme to resolve the exponential behavior of the distribution function. This scheme enhances the diagonal elements of the discrete coefficient matrix, and helps to numerically account for the rapid variation in the distribution function. With this approach, $f_0(\varepsilon,x)$ is expressed as the Slotboom-like form

$f_0(\varepsilon, x) = n(x)q(\varepsilon, x)$; and $n(x)$ is given as $n_i u(x) \exp(\phi(x)/V_t)$. We then substitute these new variables into the symmetrical and antisymmetrical equations obtained from the original BTE, and discretize using finite differences. We next analytically integrate the rapidly varying part of the difference equations between grid points. This allows us to account for the exponential variation of the distribution function analytically, thereby alleviating the computer of much of the burden. The discretization is then completed to yield a matrix equation with significantly enhanced diagonal terms. This discrete version of the BTE is then solved using SOR-type iterations in the real-space domain and sparse-matrix Gaussian elimination in energy-space.

3. *Self-Consistently Solving the Coupled System*

With a robust method for solving the BTE developed, the entire coupled Boltzmann-Poisson-Continuity nonlinear system is solved using a Gummel-type iteration scheme. The Poisson equation is directly discretized and solved with sparse matrix algebra. The hole-current-continuity equation is discretized with the standard Scharfetter-Gummel approach, and solved directly with sparse matrix Gaussian elimination. To facilitate convergence of the overall scheme, special damping and weighting factors have been developed which help to guide each Gummel iteration toward the proper solution. The flow chart of this numerical procedure is shown in Fig. 1.

V. Results

Simulation results of a submicron $n^+/p/n^-/n^+$ BJT are shown in Figs. 2 to 8. In Fig. 2 the prototype BJT structure is shown. Fig. 3 shows the distribution function for the entire device. In Figs. 4 and 5 we show calculated values for average velocity, carrier concentration, average energy and electric field. The figures also show that good agreement with MC calculations, which employ the same transport model, was obtained. It is worth noting that velocity overshoot, which is characteristic of non-equilibrium electron transport, is observed near the p/n^- junction. To demonstrate the robustness of the algorithm, in Figs. 6 to 8 we show results of average energy and velocity, as well as ionization coefficients, calculated for a large range of applied biases.

VI. Conclusion

We have developed an accurate and stable approach to BJT simulation by the direct, self-consistent solution to the Poisson, hole-continuity and electron-Boltzmann equations. The method calculates the distribution function for the entire device. Furthermore, the method uses less than 1/100 the CPU time required by similar MC calculations.

References

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[2] H. Lin, N. Goldsman and I.D. Mayergoyz, *Solid-State Electronics*, vol. 35, p. 769 (1992).

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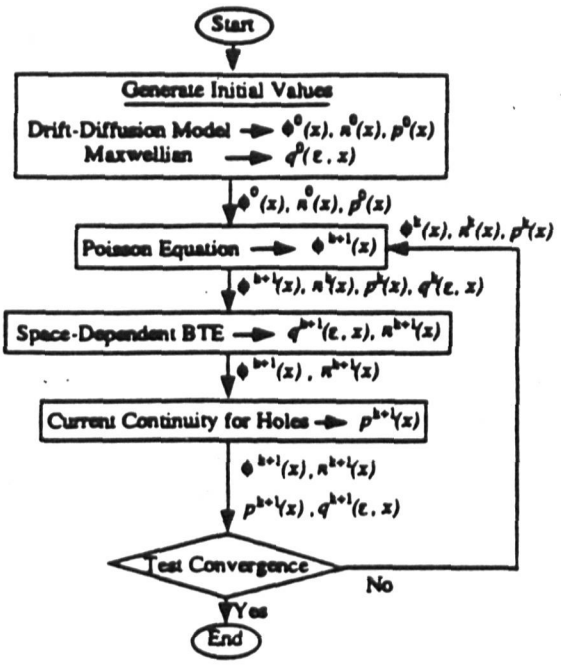


Fig. 1. The flow chart illustrates the Gummel algorithm used in this work.

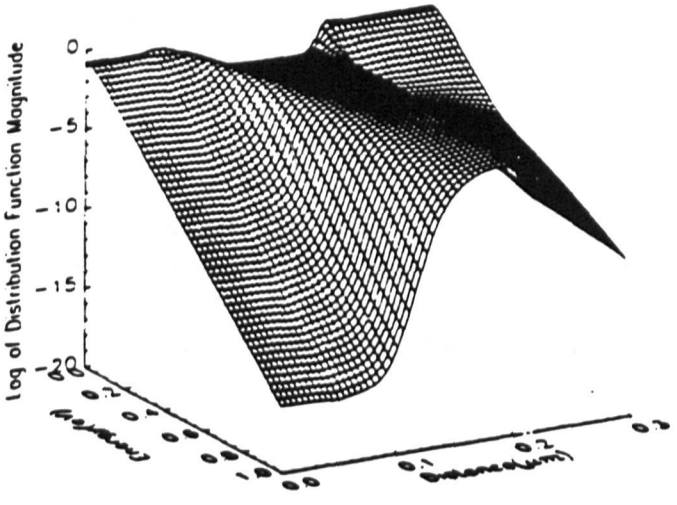


Fig. 3. The energy distribution function as a function of position along the BJT.

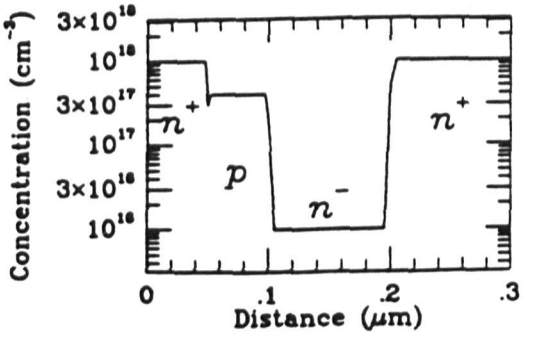


Fig. 2. The prototype BJT modeled by direct solution of the Boltzmann-Poisson-Continuity system.

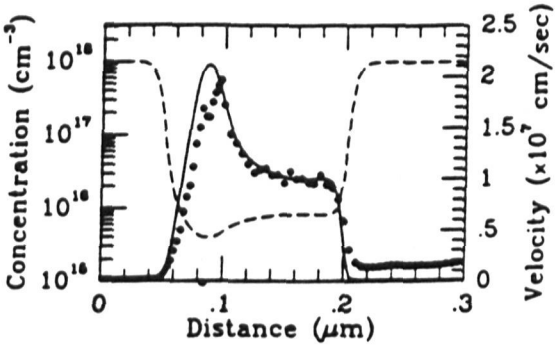


Fig. 4. Electron concentration (dash line) and average velocity (solid line) calculated by the new method. Average velocity from MC calculations (open circles) is also plotted.

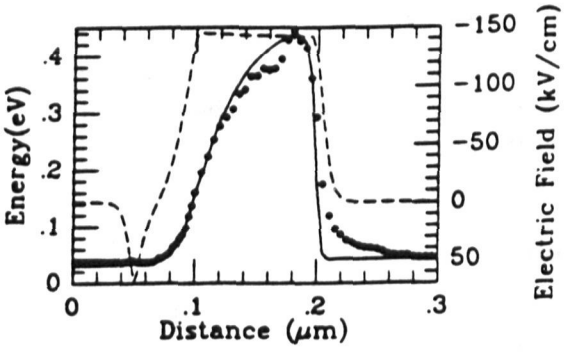
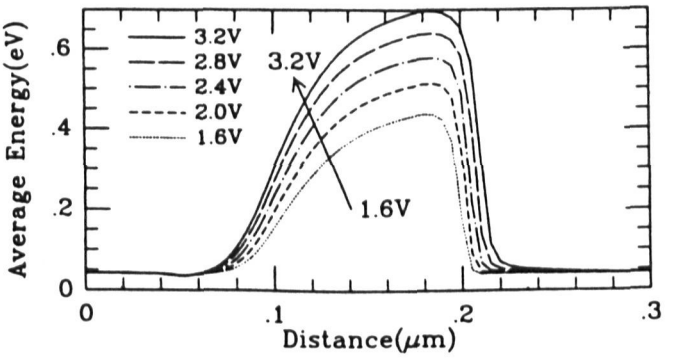


Fig. 5. Electric field (dash line) and average energy (solid line) calculated with this direct method. MC calculations are also plotted (open circles).

Fig. 6. Average electron energy as a function of position along the BJT. The simulations easily converge for a wide range of applied biases using the Scharfetter Gummel-like discretization of the Boltzmann-Poisson-Continuity system.



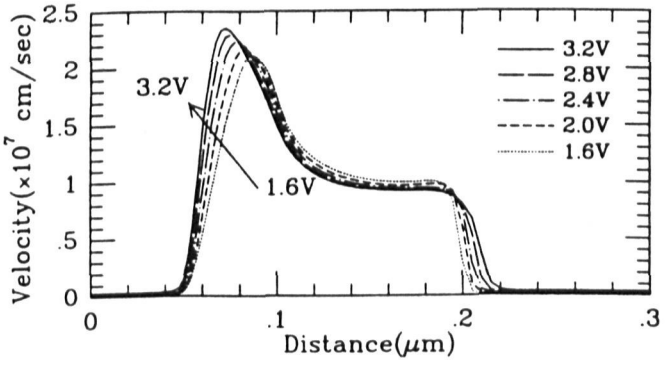


Fig. 7. Average electron velocity as a function of position calculated by the Boltzmann-Poisson-Continuity system for a wide range of applied biases. Velocity overshoot is clearly predicted by the method.

Fig. 8. Values for impact ionization coefficient calculated for a wide range of applied bias voltages. It is clear that impact ionization is maximum in the high-field collector region.