2-D MOSFET Simulation by Self-Consistent Solution of the Boltzmann and Poisson Equations Using a Generalized Spherical Harmonic Expansion

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Abstract

MOSFET simulation is performed by direct self-consistent solution of the Boltzmann, Poisson and Hole Continuity equations. To formulate the Boltzmann equation, a spherical harmonic approach has been developed which allows for expansion to arbitrarily high order. The self-consistent 2-dimensional MOSFET simulations incorporated four spherical harmonics. Simulation results provide the distribution function for the entire device, as well as substrate current, and average quantities including electron temperature, average velocity, and carrier concentration.

1. Introduction

The Spherical Harmonic approach to solving the Boltzmann equation is being demonstrated as a viable approach to device simulation[1, 2, 3]. We present here a new 2-D MOSFET simulation tool which employs a spherical harmonic expansion to deterministically solve the Boltzmann transport equation (BTE). The unique aspects of the approach are: (i) The spherical harmonic formulation of the BTE is performed to arbitrarily high order; (ii) A Scharfetter-Gummel type discretization has been developed for the BTE; (iii) Self-Consistent solution of the BTE, Poisson and Hole Continuity equations is achieved for the 2-D MOSFET structure; (iv) Results provide the electron distribution function, electrostatic potential and hole-concentration for the entire device; (v) From the distribution function, average quantities including electron temperature, average velocity, carrier concentration, as well as substrate current resulting from impact ionization, are obtained.

2. The Device Model

Our simulator is based on the following device model which consists of the Poisson equation, the BTE for electrons and the current-continuity equation for holes:

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

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

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

where: $f(\mathbf{k},\mathbf{r})$ is the distribution function; $n(\mathbf{r}) = \frac{1}{4\pi^3}\int f(\mathbf{k},\mathbf{r})d\mathbf{k}$ is the electron concentration; $p(\mathbf{r})$ is the hole concentration; $\phi(\mathbf{r})$ is the potential; We incorporate a nonparabolic band-structure, as well as acoustic, optical and intervalley phonon scattering, and impact ionization.

3. Formulation of the 2-D BTE to Arbitrarily High-Order

For steady-state 2-D MOSFET simulation, the BTE is a 5-dimensional integro-differential equation, and is therefore extremely difficult to solve. Using the SH expansion method, the BTE is reduced into a 3-dimensional system of differential-difference equations which is tractable for MOSFET simulation. We also employ the Hamiltonian transformation[3]. In contrast to other recent works, which were based on a low order SH expansion[1, 3], we have generalized the expansion approach and formulated the BTE to arbitrarily high-order SH accuracy[2]. With this approach, the momentum distribution function is expressed in terms of an infinite series of spherical harmonics: $f(\vec{r},\vec{k}) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} f_l^m(\vec{r},\varepsilon)Y_l^m(\theta,\phi)$. Where $f_l^m(\vec{r},\varepsilon)$ represent the unknown expansion coefficients; and the spherical harmonics basis functions $Y_l^m(\theta,\phi)$ provide the angular dependence of the distribution function. To determine the coefficients, $f_l^m(\vec{r},\varepsilon)$, we first substitute the above summation into the BTE. Next, we project the BTE onto each of the SH basis functions:

$$\int_0^{2\pi} d\phi \int_{-1}^{1} d(\cos\theta) Y_l^{m*}(\theta,\phi)\left\{\frac{\partial f}{\partial t} + \vec{v}\cdot\frac{\partial f}{\partial \vec{x}} + (-q)\vec{E}\cdot\frac{\partial f}{\partial \vec{p}} - \left[\frac{\partial f}{\partial t}\right]_c\right\} = 0 \ . \tag{4}$$

By performing a similar projection onto each of the SH basis functions, an infinite system of coupled equations is generated for the unknown coefficients. We then take advantage of the SH recurrence relations to facilitate performing the projections indicated by Eqn. (4). The interesting result is that almost all of the infinite terms in each equation vanish identically due to orthogonality, and the coupling between equations is only through neighbors. Another extremely useful result is that each equation has an identical form. The system can therefore be automatically generated to arbitrarily high order and then be solved numerically. The equation for the l,m SH coefficient is given below. The equation for any of the other SH coefficients is obtained by simply appropriately changing the value of the indices l,m to other allowed integers:

$$\left\{\sum_{i=1}^{2} v(\varepsilon)\left[\frac{\partial}{\partial x_i} - eE_i\left(\frac{\partial}{\partial\varepsilon} - \frac{l-1}{2}\frac{\gamma'}{\gamma}\right)\right]\hat{a}_i^+ + v(\varepsilon)\left[\frac{\partial}{\partial x_i} - eE_i\left(\frac{\partial}{\partial\varepsilon} + \frac{l+2}{2}\frac{\gamma'}{\gamma}\right)\right]\hat{a}_i^-\right\} f_l^m$$

$$= \left[\frac{\partial f_l^m}{\partial t}\right]_c \tag{5}$$

where $v(\varepsilon) = \sqrt{2m\gamma}/m\gamma'$, $\gamma' = d\gamma/d\varepsilon$, and γ represents the dispersion relation; the sum is over the 2 directions in the $x-z$ plane; and we have constructed the operators $\hat{a}$ to relate nearest-neighbor coefficients with the following definitions:

$$\hat{a}_1^+ f_l^m \equiv \frac{1}{2}\left\{-\alpha_{l-1}^m \alpha_l^m f_{l-1}^{m-1} + \alpha_{l-1}^{-m} \alpha_l^{-m} f_{l-1}^{m+1}\right\}$$
$$\hat{a}_1^- f_l^m \equiv \frac{1}{2}\left\{\alpha_{l+1}^{-m+1} \alpha_l^{-m+1} f_{l+1}^{m-1} + \alpha_{l+1}^{m+1} \alpha_l^{m+1} f_{l+1}^{m+1}\right\}$$
$$\hat{a}_2^+ f_l^m \equiv \alpha_{l-1}^{-m+1} \alpha_l^m f_{l-1}^m; \qquad \hat{a}_2^- f_l^m \equiv \alpha_{l+1}^m \alpha_l^{-m+1} f_{l+1}^m; \qquad \alpha_l^m = \sqrt{\frac{l+m}{2l+1}}$$

4. Numerical Approach to 3-D Problem

To solve the SH-expanded BTE for a 2-D MOSFET we use eqn. (5) to generate equations for the first 4 spherical harmonics. Next, we reduce these 4 equations into one second order self-adjoint differential-difference equation similar to that of[3]. We then perform a Scharfetter-Gummel type discretization on the resulting equation. This yields a matrix which is well conditioned. We overcome problems typically associated with 3-dimensional calculations by using a fixed point SOR iterative solution technique. This method avoids direct solution of large matrix equations (and is easily parallelized). The Poisson equation is solved directly in 2-D using Gaussian elimination for banded matrices. The Hole-Continuity equation is solved using Slotboom variables and the fixed point iterative method. The Boltzmann-Poisson-Hole-Continuity system is solved self-consistently using a decoupled Gummel-type iterative process.

5. Simulation Results for a 2-D MOSFET

We performed example calculations on a $0.5\mu m$ channel length nMOSFET. We show example results for an applied bias of $V_{ds} = 3V$ and $V_{gs} = 3V$. Fig. 1 shows the resulting electrostatic potential which has been calculated self-consistently with the distribution function. In Fig. 2, the electron concentration within the device, which is obtained by numerical integration of the distribution function, has been plotted. Fig. 3 shows the energy distribution function along a plane at $0.001\mu m$ below the Oxide/Si interface. It can be easily seen, by the distribution function's non-Maxwellian form, that electrons were heated up when traveling toward the drain region. This quantifies the hot-electron concentration at the channel/drain edge, which is the region that generates reliability problems. Fig. 4 shows the distribution function along a plane in the substrate. Clearly, the distribution function is Maxwellian at this depth in the device since current densities and fields are very small. Fig. 5 shows the concentration of electrons and holes generated per second by impact ionization. These values are obtained by directly integrating the impact-ionization collision term in the BTE. Fig. 6 shows the substrate current as a function of applied bias. The curves were obtained by integrating the impact-ionization collision term over the entire energy and real space domain.

References

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[3] A. Gnudi, D. Ventura, G. Baccarani, and F. Odeh, "Two-Dimensional MOSFET Simulation by means of a Multidemensional Spherical Harmonics Expansion of the Boltzmann Transport Equation," *Solid-State Electronics*, vol. 36, p. 575, 1993.

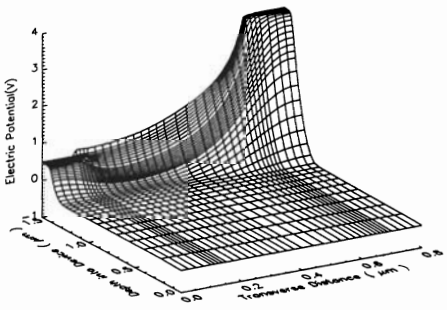

fig.1: Electric potential

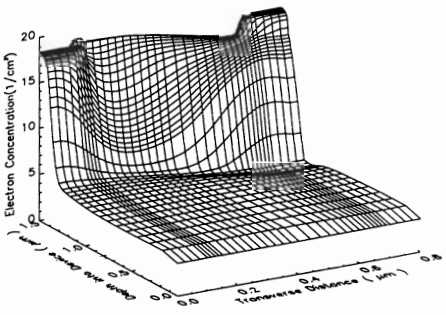

fig.2: Electron concentration

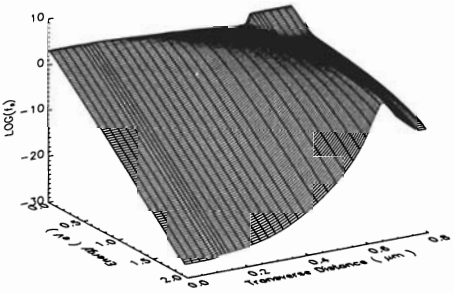

fig.3: Distribution function along the channel

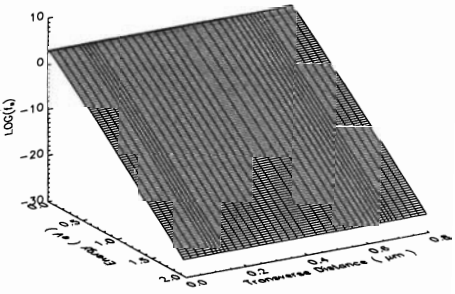

fig.4: Distribution function in substrate

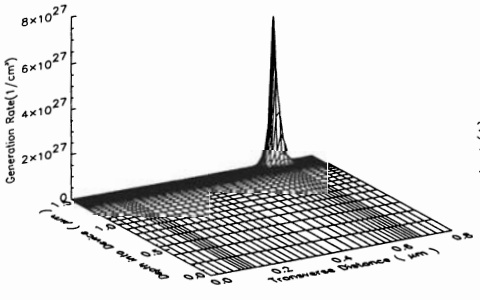

fig.5: Impact ionization generation rate

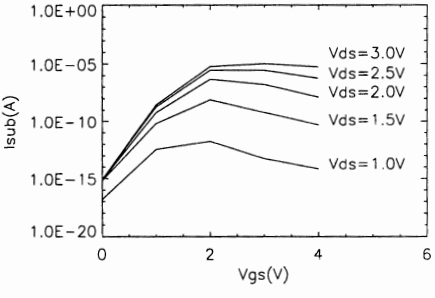

fig.6: Substrate current