SIMULATION OF n^+nn^+ CHANNEL USING FINITE DIFFERENCE TECHNIQUES FOR BOLTZMANN EQUATION

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Abstract

We simulate an n^+nn^+ silicon channel using finite difference discretization of Boltzmann Equation in one spatial dimension and two dimensional velocity space coupled to Poisson equation. The Boltzmann transport equation, BTE, is reduced to two dimensions in velocity space by assumption of density being invariant under rotations around z axis. Moments of density function are calculated numerically and compared to corresponding terms in the Hydrodynamic model. Comparisons indicate that models for viscosity and heat conduction terms are reasonable but model for momentum relaxation time does not agree well with numerical results from Boltzmann and seems to be the source of spurious overshoot in the Hydrodynamic model.

1 Introduction

Let $f(\mathbf{x}, \mathbf{u}, t)$ be the probability density function of electrons, where $\mathbf{x} = (x, y, z)$ and $\mathbf{u} = (u, v, w)$. Then the dynamics of electrons can be modeled by:

$$f_t + \mathbf{u}\nabla_{\mathbf{x}} f + \mathbf{F}\nabla_{\mathbf{u}} f = \int s(\mathbf{u}', \mathbf{u}) f(\mathbf{u}') d\mathbf{u}' - \int s(\mathbf{u}, \mathbf{u}') f(\mathbf{u}) d\mathbf{u}' \tag{1}$$

$$\nabla.(\epsilon \nabla \phi) = e(-N_D + n), \tag{2}$$

where $(F_x, F_y, F_z) = \mathbf{F} = \frac{-e}{m}\mathbf{E} = \frac{e}{m}\nabla\phi$, $s(\mathbf{u}, \mathbf{u}')$ is the scattering operator, ϕ is the electric potential, and $\mathbf{E}$ is the electric field. We use the notation $< \psi(\mathbf{u}), f >= \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} \psi(\mathbf{u}) f(\mathbf{u}) d\mathbf{u}$. From the Boltzmann equation one can obtain conservation laws of the form:

$$< \psi, f >_t + \nabla_{\mathbf{x}} < \mathbf{u}\psi, f >= \mathbf{F} < \nabla_{\mathbf{u}}\psi, f > + < \psi, S > . \tag{3}$$

By taking $\psi = m, m\mathbf{u}$, or $\frac{1}{2}m\mathbf{u}^2$ one recovers the Euler Equations of gas dynamics. These equations have been proposed by Bløtekjær [1] and have been studied numerically by many researchers. Please see [7], [4], and [5]. In the numerical calculations done in [4] velocity spikes were observed as electrons cross the channel into the drain. In this paper we try to resolve this issue.

In particular we are interested in assessing the effect of approximations for heat conduction, viscosity, and momentum relaxation terms. Please see [3] for derivation of fluid equations from the Boltzmann equation and related approximations. Define $\mathbf{v}$ to be the average velocity $\mathbf{v} = \frac{<\mathbf{u}, f>}{<1, f>}$. Then $\frac{1}{2}m < (\mathbf{u} - \mathbf{v})^3, f >\approx \kappa n \nabla T$,

$$\frac{1}{2}m < (\mathbf{u} - \mathbf{v})^2, f >= \begin{pmatrix} nT_{11} & nT_{12} & nT_{13} \\ nT_{21} & nT_{22} & nT_{23} \\ nT_{31} & nT_{32} & nT_{33} \end{pmatrix} \approx$$

[1]Regrettably Faroukh is no longer with us. His sudden death was a big loss for his family, friends, and colleagues. He will be remembered for his gentle and generous soul.

$$\begin{pmatrix} nT & 0 & 0 \\ 0 & nT & 0 \\ 0 & 0 & nT \end{pmatrix} - \nu \begin{pmatrix} \frac{4}{3}u_x - \frac{2}{3}v_y - \frac{2}{3}w_z & u_y + v_x & w_x + u_z \\ u_y + v_x & \frac{4}{3}v_y - \frac{2}{3}u_x - \frac{2}{3}w_z & w_y + v_z \\ u_z + w_x & v_z + w_y & \frac{4}{3}w_z - \frac{2}{3}u_x - \frac{2}{3}v_y \end{pmatrix}$$

Temperature is defined as $T = T_{11} + T_{22} + T_{33}/3$ and $\nu = \tau_p nT$ is the coefficient of viscosity. $< \mathbf{u}S, f > \approx \frac{-<\mathbf{u}, f>}{\tau_p}$, where τ_p is the momentum relaxation time. We use the results from BTE code to verify the models for ν, κ, and τ_p, where $\kappa = \frac{3\mu_0 k_b^2 T_0}{2e}$, and $\tau_p = \frac{m\mu_0 T_0}{eT}$ [2].

2 Transformation to Polar Coordinates

In this paper we consider a case where electric field is in the z axis direction. This implies that problem is invariant under rotations around z axis. Exploiting this property we do a coordinate transformation in the velocity space. This enables us to reduce the number of independent variables in the velocity space from three to two. Consider the Boltzmann equation for $f(x, y, z, u, v, w, t)$. Then consider the polar transformation (k, θ, ϕ) to (u, v, w) via: $u = k\sin\theta\cos\phi$, $v = k\sin\theta\sin\phi$, and $w = k\cos\theta$. Assume f is only dependent on z, k, θ, t, and introduce a new variable $\mu = \cos\theta$. The reduced system is:

$$f_t + k\mu f_z + F_z\{\mu f_k + \frac{2\mu f}{k} + \frac{((1-\mu^2)f)_\mu}{k}\} =$$
$$2\pi \int\int s(k', \mu', k, \mu) f(k', \mu') k'^2 dk' d\mu' - 2\pi \int\int s(k, \mu, k', \mu') f(k, \mu) k'^2 dk' d\mu' \tag{4}$$

$$\phi_{zz} = \frac{e}{\epsilon}(n - N_D), \tag{5}$$

where $n = 2\pi \int\int f(k, \mu) k^2 dk d\mu$, and $F_z = \frac{e}{m}\phi_z$. The system is completed with initial value and boundary conditions. We considered only the following scattering terms: $s(\mathbf{u}, \mathbf{u}') = s_{ac}(\mathbf{u}, \mathbf{u}') + s_{op}^{em}(\mathbf{u}, \mathbf{u}') + s_{op}^{abs}(\mathbf{u}, \mathbf{u}')$, where $s_{ac}(\mathbf{u}, \mathbf{u}') = \frac{1}{(2\pi)^3}(\frac{m}{\hbar})^3 \frac{2\pi k_B T_0 E_{ac}^2}{\hbar u_l^2 \rho} \delta[E(\mathbf{u}') - E(\mathbf{u}))]$, $s_{op}^{em}(\mathbf{u}, \mathbf{u}') = \frac{1}{(2\pi)^3}(\frac{m}{\hbar})^3 \frac{\pi (D_t K)^2}{\rho\omega_{op}} N_{op}^+ \delta[E(\mathbf{u}') - E(\mathbf{u}) + \hbar\omega_{op}]$, and $s_{op}^{abs}(\mathbf{u}, \mathbf{u}') = \frac{1}{(2\pi)^3}(\frac{m}{\hbar})^3 \frac{\pi (D_t K)^2}{\rho\omega_{op}} N_{op} \delta[E(\mathbf{u}') - E(\mathbf{u}) - \hbar\omega_{op}]$. E is energy of an electron and is given by $E(\mathbf{u}^2) = \frac{1}{2}m\mathbf{u}^2 = \frac{1}{2}mk^2$, $N_{op} = \frac{1}{e^{\frac{\hbar\omega_{op}}{k_B T_0}} - 1}$, and $N_{op}^+ = N_{op} + 1$.

3 The Ballistic Diode Problem

As a model problem, we simulate the flow of electrons in a submicron n^+nn^+ silicon diode. This device models the channel in a MOSFET. The diode begins with an n^+ "source" region, is followed by an n "channel" region, and ends with an n^+ "drain" region. The effects of holes may be neglected for the ballistic diode problem. For a discussion of the proper constants and units we refer the reader to (Fatemi-Jerome-Osher) [4].

4 Numerical Scheme

The numerical scheme used in these calculations uses explicit time stepping and upwind finite differences. Let us define a grid in (z, k, μ, t) space. Let $f_{sij}^n = f(s\Delta z, i\Delta k, , j\Delta\mu, n\Delta t) = f(z_s, k_i, \mu_j, t_n)$.

Then define backward differences as $D_z^- f_{sij} = (f_{sij} - f_{s-1i,j})/\Delta z$, forward differences as $D_z^+ f_{sij} = (f_{s+1,ij} - f_{sij})/\Delta z$, and central differences as $D_z^0 f_{sij} = (f_{s+1,ij} - f_{s-1,ij})/2\Delta z$. The numerical scheme is:

$$D_z^+ D_z^- \phi_s^n = \frac{e}{\epsilon}(n_s - n_{Ds}) \quad F_s = \frac{e}{m} D_z^0 \phi_s \tag{6}$$

$$\frac{f^{n+1} - f^n}{\Delta t} + k\mu \frac{\hat{f}_{s+\frac{1}{2}} - \hat{f}_{s-\frac{1}{2}}}{\Delta z} + F_z\{\mu \frac{\hat{f}_{i+\frac{1}{2}} - \hat{f}_{i-\frac{1}{2}}}{\Delta k} + \frac{2\mu \bar{f}_i}{k} + \frac{\hat{g}_{j+\frac{1}{2}} - \hat{g}_{j-\frac{1}{2}}}{k\Delta\mu}\} = S_{sij}. \tag{7}$$

Define $\bar{f}_i = \frac{\hat{f}_{i+\frac{1}{2}} + \hat{f}_{i-\frac{1}{2}}}{2(1+\frac{\Delta k^2}{4k^2})}$ and $n_s = 2\pi \sum_j \sum_i (k_i^2 + \frac{\Delta k^2}{4}) f_{sij} \Delta k \Delta\mu$. The definitions for n_s and $\bar{f}$ are chosen such that in each time step mass is conserved. Flux functions $\hat{f}_{s+\frac{1}{2}}$, $\hat{f}_{i+\frac{1}{2}}$, and $\hat{g}_{j+\frac{1}{2}}$ are defined in upwind fashion: $\hat{f}_{s+\frac{1}{2}} = f_s$ if $k\mu > 0$, $\hat{f}_{s+\frac{1}{2}} = f_{s+1}$ if $k\mu < 0$, $\hat{f}_{i+\frac{1}{2}} = f_i$ if $F_z\mu > 0$, $\hat{f}_{i+\frac{1}{2}} = f_{i+1}$ if $F_z\mu < 0$, $\hat{g}_{j+\frac{1}{2}} = (1-\mu^2) f_j$ if $F_z > 0$, and $\hat{g}_{j+\frac{1}{2}} = (1-\mu^2) f_{j+1}$ if $F_z < 0$. The scattering terms, S_{sij}, were calculated using the trapezoidal rule. The scattering term s_{ac} was analytically integrated in the k space. For integrating s_{op}^{em} and s_{op}^{abs} an approximation to the δ function was used.

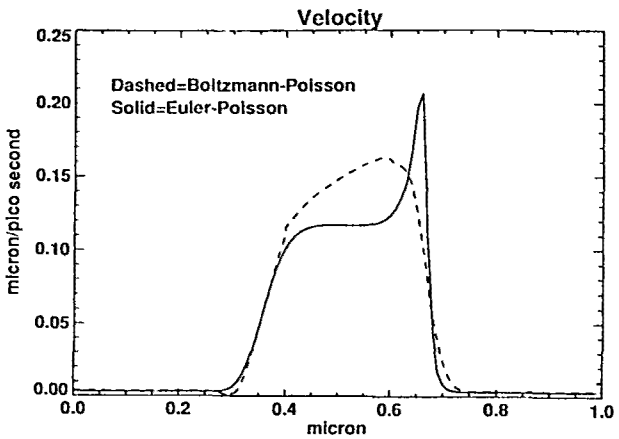

Figure 1 Electron Velocity

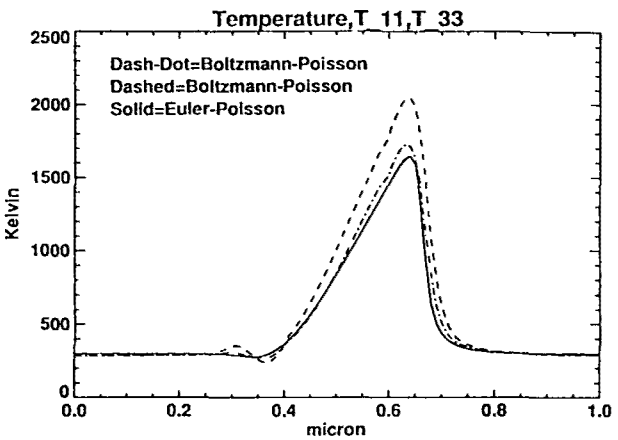

Figure 2 Temperature(Hydro), T_{11}, and T_{33}

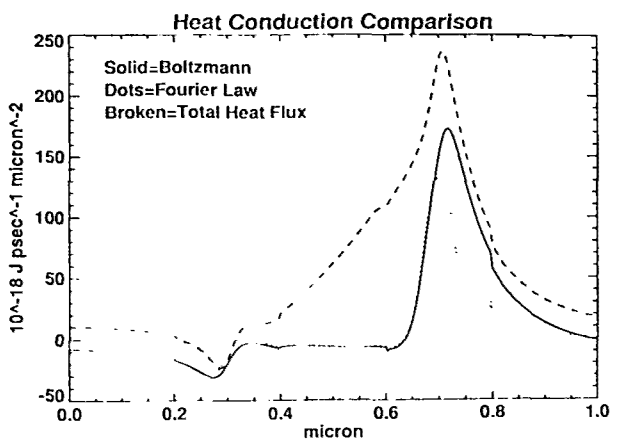

Figure 3 Heat Conduction Comparison

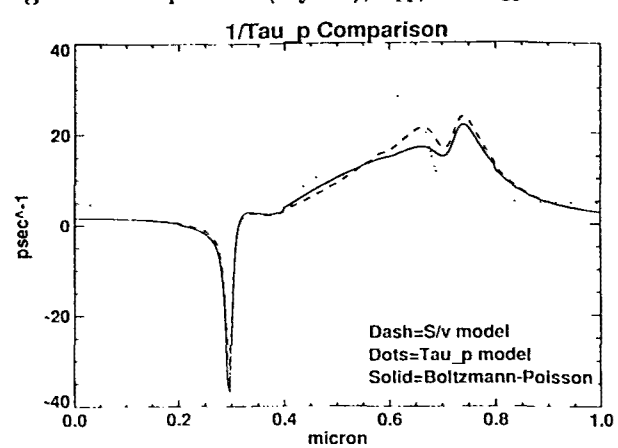

Figure 4 Momentum Relaxation Time

Since this is an explicit time stepping, the time steps have to be limited to satisfy the Courant-Friedrichs-Lewy condition. In computations an automatic time step was chosen based on the CFL

criteria and no instability was observed.

5 Numerical Results and Conclusion

In figure one we show the calculated velocities from the Boltzmann and Hydrodynamic codes. Note that the spike is missing in the Boltzmann solution. In figure two we compare the calculated temperatures from the Hydro model and the BTE code. T_{33} is a little higher than $T_{11}(T_{11} = T_{22})$. The difference can be approximated by viscosity terms and it turns out that these terms are small and can be neglected. Calculations were done with viscosity terms included in the Hydro model and they had little effect on the velocity profile. In figure three the solid line shows the heat conduction term from the BTE and the doted line shows the heat conduction term calculated from the Fourier law, $\kappa n T_z$. For κ we use the Wiedmann-Franz law [2]. As can be seen the approximation is reasonable except in the drain.

In the last figure we plot τ_p as calculated from the BTE solution , the model suggested by Baccarni and Wordeman [2], and the model suggested by S. Lee [6]. The unusual dips in the solid line at $z = .3$ and $z = .7$ are from numerical inaccuracies. The first model for τ_p is not accurate. The second model matches the BTE better. Two features are certain. The dependence of τ_p on $\frac{1}{T}$ is too strong. The other feature is that as electrons enter the channel, relaxation of high velocity electrons requires some distance. This distance seems to be shorter for relaxation of the second moment (Temperature) but longer for the first moment of the scattering term and the third moment of the density (Heat Conduction term).

The computer time was modest for one dimensional case. For extension to two or three dimensions a more efficient algorithm is needed. These calculations indicate that models for heat conduction and viscosity are adequate. Viscosity has small effect on the flow and can be neglected. The model for τ_p is not accurate and is source of the spurious overshoot in velocity profile.

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