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Formulation of the Boltzmann Equation as a Multi-Mode Drift-Diffusion Equation

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We present a multi-mode drift-diffusion equation as reformulation of the Boltzmann equation in the discrete momentum space. This is shown to be similar to the conventional drift-diffusion equation except that it is a more rigorous solution to the Boltzmann equation because the current and carrier densities are resolved into M×1 vectors, where M is the number of modes in the discrete momentum space. The mobility and diffusion coefficient become M×M matrices which connect the M momentum space modes. This approach is demonstrated by simulating electron transport in bulk silicon.

Keywords: Semi-classical Boltzmann equation, non-equilibrium transport, multi-mode drift-diffusion

1 INTRODUCTION

With the continued down-scaling of semiconductor devices, there is a need to develop device simulators that can treat carrier transport taking into account off-equilibrium carrier distributions by solving the Boltzmann Transport Equation as accurately as possible. Several techniques have been developed to do so – such as the Monte Carlo [1], hydrodynamic [2], spherical harmonic [3], and cellular automata methods [4], and the Scattering Matrix Approach [5, 6, 7]. Each method has its own limitations – for example, computational burden, calibration of parameters, low order approximation for the distribution function, "artificial diffusion" of carriers and restriction to fixed spatial square grids. Ideally, a simulation method should provide all the capabilities of drift-diffusion simulators (i.e., simulations from equilibrium to high bias with smooth results at low computational burden) while also resolving carrier distribution and treating scattering processes rigorously. Our objective in this paper is to take a step in this direction.

Therefore, here we will describe a re-formulation of the scattering matrix equations which expresses the 1-D spatial Boltzmann equation as a 1-D spatial drift-diffusion equation in a discretised 3-D momentum space. The current and carrier densities generalise to M×1 vectors, where

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M is the number of modes in the discrete 3-D momentum space. The mobility and diffusion coefficient become M×M matrices which connect the M momentum space modes. Solving the Boltzmann equation, then, reduces to solving a set of M coupled drift-diffusion equations which might be done by a generalisation of the standard techniques for solving the conventional drift-diffusion Equation [8].

2 FORMULATION OF THE MULTI-MODE DD EQUATION

The one-mode method of McKelvey [9, 10] and similar observations by Shockley [11] can be generalised to M-modes in 3-D momentum space and this gives us an expression for the differential flux equations in 1-D real space for the M-modes in momentum space as follows [7]

$$\begin{pmatrix} \frac{d}{dx}\overrightarrow{J^+}(x) \\ \frac{d}{dx}\overrightarrow{J^-}(x) \end{pmatrix} = \begin{bmatrix} -[\xi_{11}(x)] & [\xi_{12}(x)] \\ -[\xi_{21}(x)] & [\xi_{22}(x)] \end{bmatrix} \begin{pmatrix} \overrightarrow{J^+}(x) \\ \overrightarrow{J^-}(x) \end{pmatrix}, \tag{1}$$

where the M×1 vectors $\overrightarrow{J^+}(x)$ and $\overrightarrow{J^-}(x)$ are the fluxes discretised in positive and negative directions of momentum p_x respectively, at a position x.

The elements of the (M×M) differential matrices $[\xi_{ij}(x)]$ can be interpreted as the inverse of an *inter-mode* mean free path in presence of all possible scattering mechanisms. In general, these terms can be difficult to calculate analytically and therefore we use an indirect procedure. The space-independent differential $[\xi_{ij}]$ matrices are calculated from the matrix logarithm of the transmission matrix of a semiconductor slab divided by the slab thickness. The transmission matrix itself is obtained from the scattering matrix calculated by Monte Carlo techniques [7]. All possible information about the underlying physics of scattering (band structure, phonons, ionised impurities and electric field) that is included in the Monte Carlo simulation is automatically embedded in the scattering matrix and hence in the $[\xi_{ij}]$ matrices.

Now returning to Eq. (1), we find its symmetric and anti-symmetric components and relate each flux $J_i(x)$ to its velocity v_i and its population density $n_i(x)$. Thus, we obtain a multi-mode drift-diffusion equation and its associated continuity equation:

$$\vec{J}(x) = e[\mu(x)]\vec{n}(x)\mathcal{E}_x + e[D(x)]\frac{d}{dx}\vec{n}(x), \tag{2}$$

$$\frac{d}{dx}\vec{J}(x) = [\alpha(x)]\vec{J}(x) + [\beta(x)]\vec{n}(x), \tag{3}$$

where the diffusion, inverse Einstein and mobility matrices are defined as follows:

$$[D(x)] = 2\{[\xi_{11}(x)] + [\xi_{12}(x)] + [\xi_{21}(x)] + [\xi_{22}(x)]\}^{-1}[\mathcal{V}], \tag{4}$$

$$[E]^{-1} = \frac{1}{2\mathcal{E}_x}\{[\xi_{11}(x)] - [\xi_{12}(x)] + [\xi_{21}(x)] - [\xi_{22}(x)]\}, \tag{5}$$

$$[\mu(x)] = [D(x)][E]^{-1}, \tag{6}$$

and $[\mathcal{V}]$ is a diagonal matrix whose elements are the mode velocities.

The coefficient matrices for the continuity equation are

$$[\alpha(x)] = \frac{e}{2}\{[\xi_{11}(x)] + [\xi_{12}(x)] - [\xi_{21}(x)] - [\xi_{22}(x)]\}, \tag{7}$$

$$[\beta(x)] = \frac{e}{2}\{[\xi_{11}(x)] - [\xi_{12}(x)] - [\xi_{21}(x)] + [\xi_{22}(x)]\}[\mathcal{V}]. \tag{8}$$

Equations (2) and (3) are the key results of the paper. Note that they are very similar to the conventional drift-diffusion form. This multi-mode drift-diffusion equation has associated M×M mobility and diffusion matrices that depend only on the scattering mechanisms and momentum space discretisation.

It is important to note that the field dependence of the relevant matrices here. The discrete form of the Boltzmann Transport Equation [7] indicates

that each of the differential $[\xi_{ij}(x)]$ submatrices are *linearly* dependent on the field, for any given orientation of the field. This relation makes the $[\mu(x)]$, $[D(x)]$, $[\alpha(x)]$ and $[\beta(x)]$ matrices straightforward to calculate once the invariant zero-field $[\xi_{ij}(x)]$ matrices and the field-coefficient matrices are known.

3 RESULTS

In this section, we present some preliminary results for $\langle 111 \rangle$ electric fields in bulk Si. A simple spherical, non-parabolic energy band structure was assumed for calculating scattering rates and the 3-D momentum space was discretised into 400 modes – 20 modes in transverse $|p_t|$ and 20 modes in longitudinal p_x (this implies 20 $\overrightarrow{J^+}$ fluxes for $+p_x$ and 20 $\overrightarrow{J^-}$ fluxes for $-p_x$). Scattering matrices were computed by Monte Carlo simulation [5–7] and the $[\xi_{ij}(x)]$ matrices were extracted using the procedure described in Section 2. Higher levels of accuracy with respect to the underlying band-structure and scattering can be attained just by using more sophisticated Monte Carlo techniques. The distribution of the carriers was assumed to be *uniform* across the modes, which is adequate to demonstrate proof-of-concept here.

Having obtained the $[\xi_{ij}(x)]$ matrices, we then calculated the mobility and diffusion matrices and examined their structure. These are shown in Figure 1. Calculating these matrices involves taking matrix logarithms and inverses which produces a large number of elements that are numerically near zero. If we ignore these small elements, the matrices are very sparse ($\approx 1-2\%$ ignoring elements $<0.1\%$ of the largest element) and have a simple structure. The most significant elements of the mobility matrix are the diagonal elements and off-diagonal elements only where the ith mode is connected to the jth mode by field shift. The diffusion matrix is strongly *diagonal* and has significant but small off-diagonal elements only where the ith mode is connected to the jth mode by scattering.

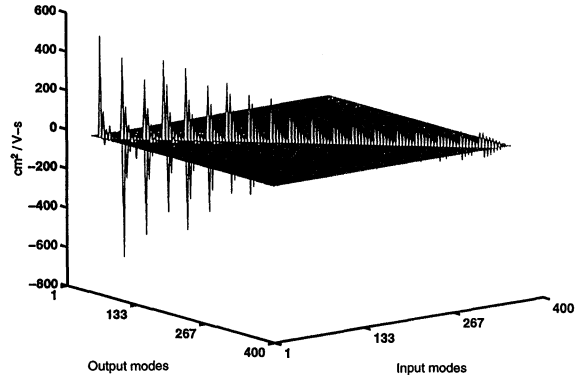

FIGURE 1a Mobility matrix for Si, non-parabolic spherical bands, 20 modes in longitudinal p_x (20 positive and 20 negative fluxes) and 20 modes in transverse $|p_t|$, $\langle 111 \rangle$ -1×10^4 V/cm.

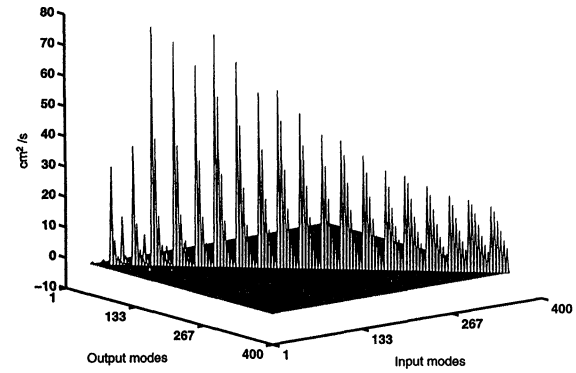

FIGURE 1b Diffusion matrix for Si, non-parabolic spherical bands, 20 modes in longitudinal p_x (20 positive and 20 negative fluxes) and 20 modes in transverse $|p_t|$, $\langle 111 \rangle$ -1×10^4 V/cm.

In order to test the formulation, we used the above matrices to simulate electron transport in bulk Si with $\langle 111 \rangle$ electric fields. The solution in bulk is simple because there are no spatial gradients in Eqs. (2) and (3). Substituting the expressions for $[\alpha]$, $[\beta]$ and $[\mu]$ from Eqs. (7), (8) and (6) respectively, we get

$$\begin{bmatrix} -[\xi_{11}] & [\xi_{12}] \\ -[\xi_{21}] & [\xi_{22}] \end{bmatrix} \begin{bmatrix} [\mathcal{V}] & [0] \\ [0] & [\mathcal{V}] \end{bmatrix} \begin{pmatrix} \overrightarrow{n^+} \\ \overrightarrow{n^-} \end{pmatrix} = \begin{pmatrix} \vec{0} \\ \vec{0} \end{pmatrix}, \quad (9)$$

which could also have been obtained directly from the differential flux Eq. (1).

The solution for the above Eq. (9) is a straightforward solution to a null-space problem (using svd factorisation in MATLAB) and it gives us the complete bulk carrier distribution function for any field $\mathcal{E}_x$. Some calculated bulk distributions for $\langle 111 \rangle$ electric fields are shown in Figure 2. Taking the average of the mobility and the diffusion matrices over the carrier distributions so obtained in the bulk,

$$\langle \mu \rangle = \frac{1}{\Sigma_i n_i} \sum_i \sum_j \mu_{ij} n_j, \tag{10}$$

$$\langle D \rangle = \frac{1}{\Sigma_i n_i} \sum_i \sum_j D_{ij} n_j, \tag{11}$$

we recover the values of macroscopic mobility and diffusion coefficients.

Plots of the results are shown in Figure (3), and we see that macroscopic mobility, diffusion coefficients and electron temperature so obtained have the expected behaviour with electric field. The low-field mobility is $\approx 30\%$ too low because of the assumed uniform intra-mode distribution. High-field results which do not suffer from this constraint are therefore more accurate – e.g. 9.915×10^6 cm/s at -1×10^5 V/cm. Note that the field dependence of $\langle \mu \rangle$ and $\langle D \rangle$ is a consequence of the field dependence of the distribution function in this approach.

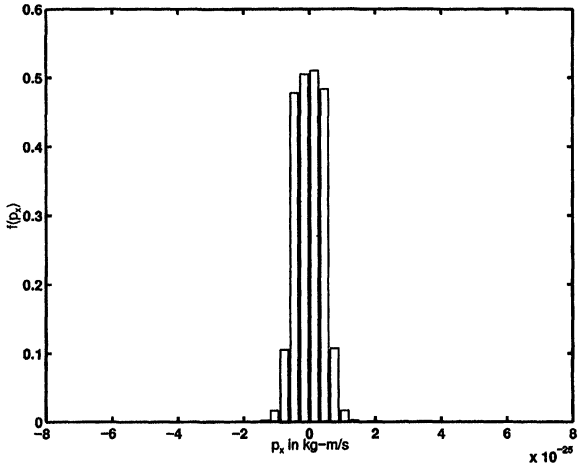

FIGURE 2a Bulk carrier distribution for $\langle 111 \rangle -1 \times 10^2$ V/cm in Si.

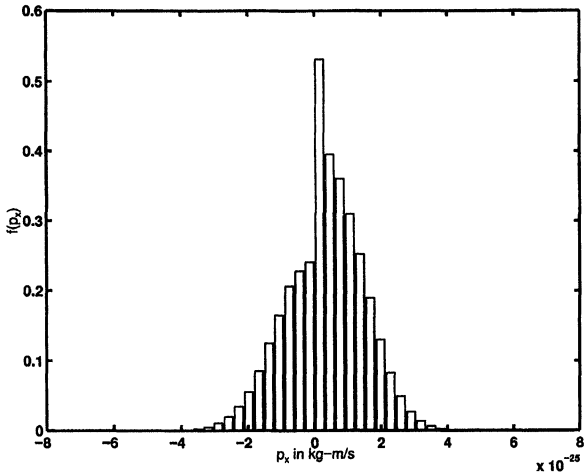

FIGURE 2b Bulk carrier distribution for $\langle 111 \rangle -1 \times 10^5$ V/cm in Si.

4 DISCUSSION

To illustrate how the equations would be solved under spatially varying conditions, we present a simple linear scheme using finite differences. By

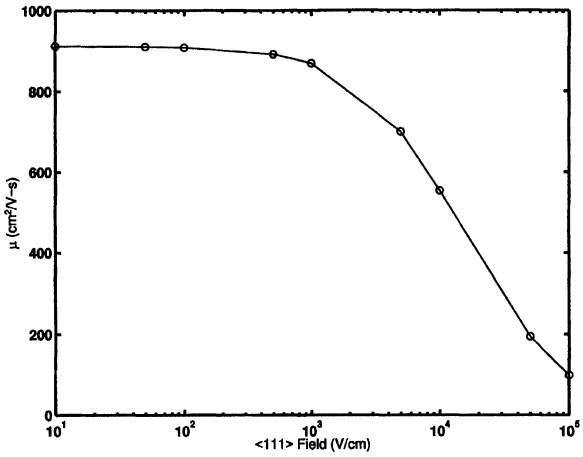

FIGURE 3a Macroscopic bulk mobility versus $\langle 111 \rangle$ electric field in Si.

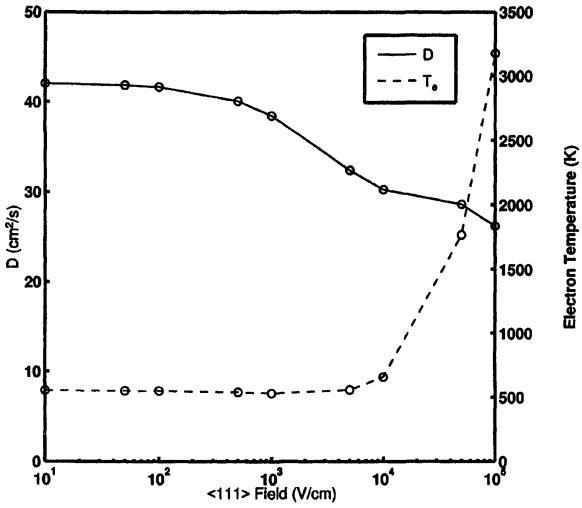

FIGURE 3b Macroscopic bulk diffusion coefficient and electron temperature (calculated from $D/\mu = k_B T_e/e$) versus ⟨111⟩ electric field in Si.

discretising $d\vec{J}(x)/dx$ on a uniform grid of size h, we obtain

$$\frac{1}{h}\left(\vec{J}\left(i+\frac{1}{2}\right)-\vec{J}\left(i-\frac{1}{2}\right)\right)=[\alpha(i)]\vec{J}(i)+[\beta(i)]\vec{n}(i), \tag{12}$$

In the simplest case, we could discretise the current equations using Eq. (2) and finite differences as follows

$$\vec{J}(i)=e[\mu(i)]\left(\frac{V(i+1)-V(i-1)}{2h}\right)\vec{n}(i) + e[D(i)]\frac{1}{2h}(\vec{n}(i+1)-\vec{n}(i-1)).$$

The result is a tridiagonal matrix form for the carrier distribution function across the device (i from 1 to N)

$$[\mathcal{L}(i-1)]\,\vec{n}(i-1)+[\mathcal{D}(i)]\,\vec{n}(i) + [\mathcal{U}(i+1)]\,\vec{n}(i+1)=\vec{0}, \tag{13}$$

where the elements of the tridiagonal matrix are now not scalars but M×M matrices and the variables are M×1 vectors. This is a large linear system whose solution is the position dependent carrier distribution function. However, the Scharfetter-Gummel method is normally the preferred scheme for discretising the conventional drift-diffusion equation because it is stable when the potential drop between adjacent nodes on a grid spacing h is greater than $2k_B T_e/e$. A corresponding result must be developed for the multi-mode semiconductor equations.

With regard to future applications, it is clear to see that finding the transitions rates for the fluxes in two (and three) spatial dimensions will give similar differential flux equations for two (and three) spatial dimensions. Therefore the multi-mode method will still hold in the most general case of transport. As a final note, we should point out that the multi-mode drift-diffusion/continuity equation formulation is formally equivalent to the differential flux equations, Eq. (1). These equations could, alternatively be integrated across the device in order to solve for carrier transport. The numerical advantages of one form over the other are not clear yet.

5 SUMMARY

To summarise, we have presented a 1-D spatial multi-mode drift-diffusion equation as reformulation of the 1-D spatial Boltzmann equation in a discrete 3-D momentum space. Although, the numerical aspects in this paper were not optimised for the best accuracy, the multi-mode drift-diffusion equation was solved in the bulk for the carrier distribution function and all the macroscopic properties that are incorporated as phenomenological models in conventional drift-diffusion were shown to fall out as a natural consequence of solving the multi-mode drift-diffusion.

The potential of this method lies in its close connection to conventional drift-diffusion – notably the equivalence of a one-mode case to conventional drift-diffusion, easy reduction to macroscopic quantities and similarity in solution

techniques. The key issue now is to formulate the problem for solution on a general 2-D spatial grid. Both deterministic and stochastic solution techniques for solving the resulting equations should be examined. From the results so far, the multi-mode drift-diffusion formulation of the Boltzmann equation promises to be a powerful approach and may overcome some of the limitations of the scattering matrix approach.

Acknowledgement

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Kausar Banoo received her B.Tech. (Electrical Engineering) from the Indian Institute of Technology, Bombay in 1993 and her M.S. (Electrical Engineering) from Duke University in 1995. Currently she is enrolled in the Ph.D. program at Purdue University and is studying scattering matrix techniques for simulating electron transport in ultra-small MOSFETs.

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Mark Lundstrom received B.E.E. and M.S.E.E. degrees from the University of Minnesota in 1973 and 1974 and a Ph.D. from Purdue University in 1980. From 1974–1977 he was employed by Hewlett-Packard where he worked on the development of a second-generation NMOS integrated circuit process. He is currently Professor of Electrical and Computer Engineering at Purdue. Lundstrom's research interests center on the physics of semiconductor devices. He is an IEEE Fellow and the recipient of the ASEE Frederick Emmons Terman Award, and of two teaching awards from Purdue University.