SCATTERING MATRIX SIMULATION OF SILICON DEVICES

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Abstract

The Scattering Matrix Approach (SMA) is a new technique for solving the Boltzmann equation in advanced devices. We first described the SMA at the 1990 Workshop on Computational Electronics and presented example calculations of electron transport in model devices [1]. Since that time, the method has been extended to treat transport in realistic devices. This paper reports on recent extensions to the SMA such as self-consistency and the development of a technique for generating single flux scattering matrices, which can be used to reproduce drift-diffusion results. Application of the technique to rigorously compute quantities such as the carrier mobility and heat flux within a device is also discussed.

I. The Approach

In the SMA, carrier transport is viewed as the transmission and reflection of carrier fluxes within a semiconductor. As shown in Figure 1, the device is represented by a set of interconnected slabs, with each slab sufficiently thin so that the doping and electric field can be considered constant within it. Transport across each slab is described by a matrix equation which relates the incident carrier fluxes to the emerging fluxes through the transmission and reflection coefficients of a scattering matrix. In order to resolve the distribution function, the flux is discretized into a number of bins in momentum space referred to as modes. The elements of the scattering matrices are computed by Monte Carlo simulation of thin slabs at constant fields. This technique consists of injecting numerous electrons into the slab within each mode and keeping track of the modes in which the electrons exit the slab [2]. In device analysis, scattering matrices for each slab in the device are cascaded and known fluxes are injected from the contacts. The fluxes through each slab are then computed iteratively until they converge. From the magnitude of the fluxes within each mode, the position dependent distribution function is constructed and transport quantities of interest can be computed. When the scattering matrix problem is solved in this manner, the SMA has recently been proven to be a solution of the spatially inhomogeneous Boltzmann equation [3].

II. Self-consistency

Previous SMA work involved non-self-consistent simulation of model structures with piece-wise constant electric fields [2]. Adding self-consistency therefore required the ability to simulate devices with arbitrary field profiles. This was accomplished by computing a library of scattering matrices at ten different fields and then interpolating a scattering matrix for each slab in the device from this library according to the the field profile. Next, in order to ensure space neutrality at the contacts, an iterative method was used to compute the correct flux injected at the contacts. This method involved treating the contacts as infinite bulk regions, which inject the same flux distribution as found in a bulk semiconductor at the boundary electric field values. After the fluxes were solved by the SMA under these conditions, the electron concentration was computed and Poisson's equation was solved to update the potential. The entire solution procedure was then iterated via Gummel's method until a self-consistent result was obtained. The convergence behavior of the SMA compared to direct Monte Carlo simulation for the potential in an n-i-n diode is shown in Figure 2(a), while the velocity in the device computed by both methods is displayed in Figure 2(b) [4]. The SMA results are shown to be much smoother, allowing better convergence.

III. Single Flux Scattering Matrices

In order to efficiently reproduce drift-diffusion results and to bridge the gap between McKelvey's flux method [5] and the multi-flux SMA, a single flux scattering matrix technique was developed. In the single flux approach, the incoming and outgoing fluxes within each slab are not resolved in momentum space, so the scattering matrices contain only four elements. At each field in the matrix library, the carrier distribution is assumed to be the bulk distribution and is characterized by the average positive velocity and the average negative velocity of the carriers. In device simulation, the magnitudes of the carrier fluxes associated with positive and negative velocities are computed by an iterative technique similar to the multi-flux SMA. Figure 3(a) shows the velocity field characteristic computed by the single flux SMA compared to Monte Carlo calculations. A similar characteristic was also computed for holes. In Figure 3(b), the self-consistent results for the velocity in the n-i-n are given from both single flux scattering matrix simulation and a drift-diffusion simulator with a field-dependent mobility and diffusion coefficient.

IV. Application for Computing Transport Quantities in Devices

Since the SMA treats semi-classical transport rigorously, it resolves the carrier distribution function throughout the device. From the distribution function, quantities such as the carrier temperature, heat flux, and average momentum relaxation time can be computed. For example, the heat flux is given by

$$Q_z(z) = \frac{1}{4\pi^3} \sum_{\mathbf{p}} \frac{1}{2} m^*(E) \left|v - v_{dz}(z)\right|^2 (v_z - v_{dz}(z))\, f(\mathbf{p},z) \ ,$$

where the distribution function $f(\mathbf{p},z)$ is determined from the magnitude of the flux associated with each mode in the descretized momentum space and the sum is over all modes. Figure 4(a) shows the diagonal z component of the carrier temperature tensor, T_{zz}, and the heat flux, $\mathbf{Q}_z$, within the n-i-n diode. The carrier temperature displays the expected result: slightly cooling in the barrier region and rising rapidly in the high field region. However, note that $\mathbf{Q}_z$ does not change sign where the peak in the electron temperature occurs, contrary to Fourier's law ($\mathbf{Q}_z = -k\nabla T$), an assumption made in many macroscopic models. From the rigorous solution for the energy and mobility shown in Figure 4(b), it is also apparent that the mobility is not a single valued function of energy. This is a result of the shape of the distribution function, which changes substantially from the increasing to decreasing field regions [6]. These results, discussed in more detail in [7], demonstrate that the SMA can be a valuable asset for examining the assumptions made in other transport models.

V. Conclusion

Self-consistency and the development of the single flux method to reproduce drift-diffusion results for holes represent important steps in creating a complete 1-D bipolar simulator based upon the Scattering Matrix Approach, a new technique for solving the Boltzmann equation in devices. The convergence behavior of the self-consistent results shows an inherent advantage of the SMA over the typically more noisy Monte Carlo technique while the single flux method demonstrates the versatility of the approach. In addition, the ability to accurately compute quantities from the distribution function throughout a device demonstrates that the SMA can be powerful technique for testing the assumptions made in macroscopic models.

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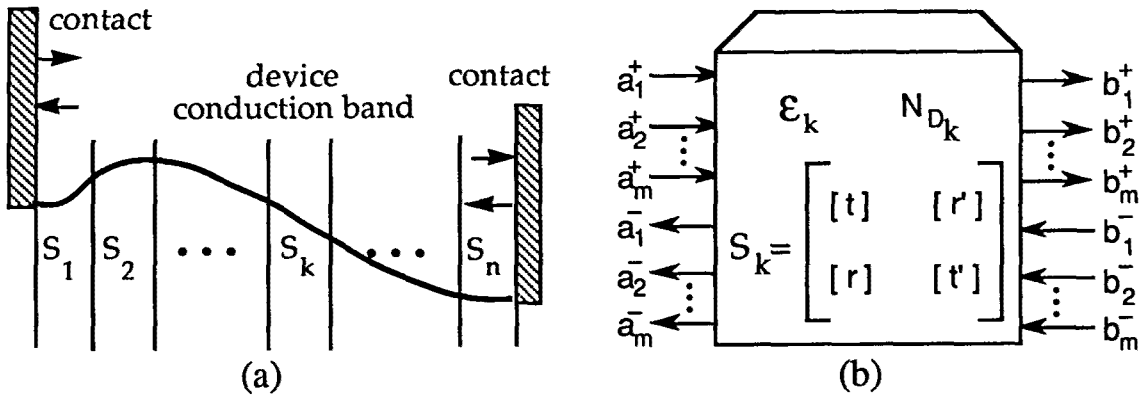

Fig 1. Basic concept of device simulation in the SMA [4]. The device is divided into slabs (a) which are each represented by a scattering matrix S_k. Each matrix models the transport of a number of carrier fluxes resolved in momentum space through the slab (b). The coefficients of S_k (t,t',r,and r') are matrices relating all of the incident and scattered fluxes .

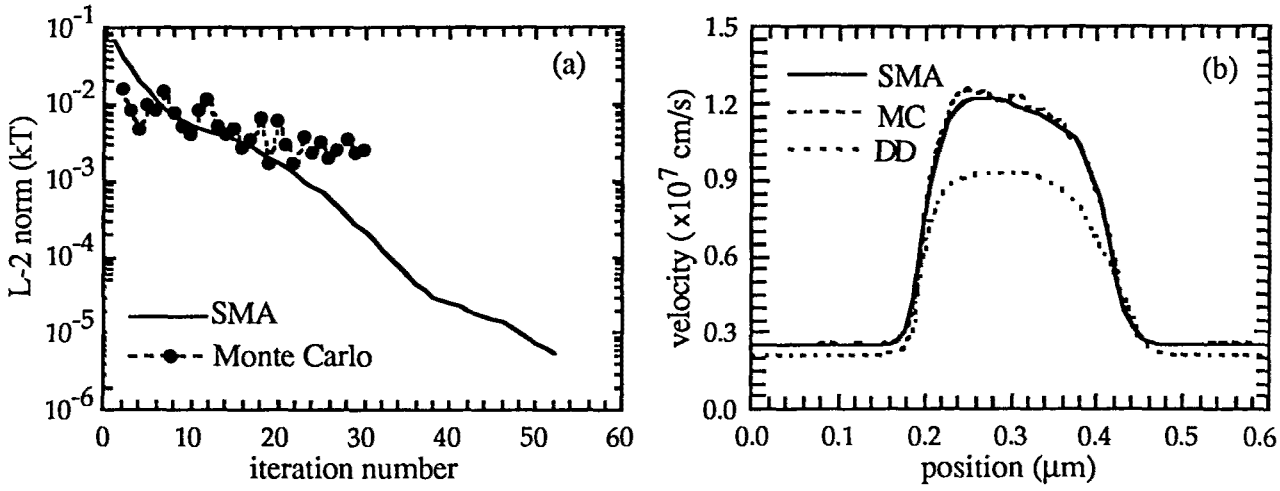

Fig 2. The device in these simulations was an n-i-n diode biased 1.5 volts. (a) The L-2 norm for the potential corrections versus number of times Poisson's equation was solved. (b) The velocity vs. position as computed by the Scattering Matrix Approach (SMA), Monte Carlo simulation (MC), and a drift-diffusion simulator (DD) with a field dependent mobility [4].

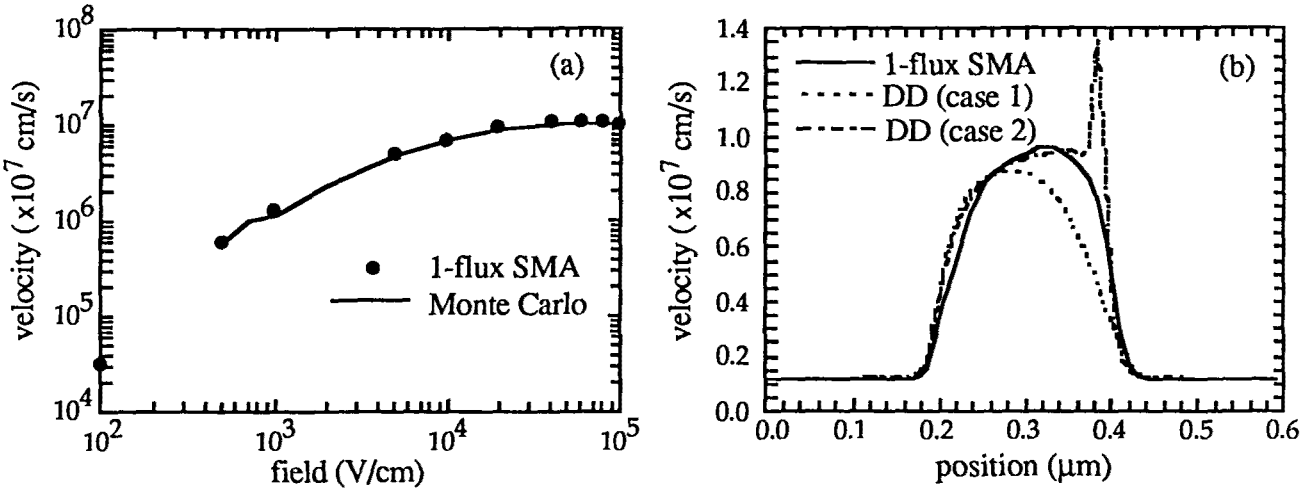

Fig 3. (a) The velocity-field characteristic computed by the single flux scattering matrix approach (1-flux SMA). (b) The velocity versus position for an n-i-n diode biased 0.75 volts. Comparison is made between the single flux scattering matrix results and a drift-diffusion simulator with a field dependent mobility and constant diffusion coefficient (case 1) and with both a field dependent mobility and field dependent diffusion coefficient (case 2). The single flux scattering matrix approach, which makes no explicit assumptions about the form of the diffusion coefficient, falls between these two limits.

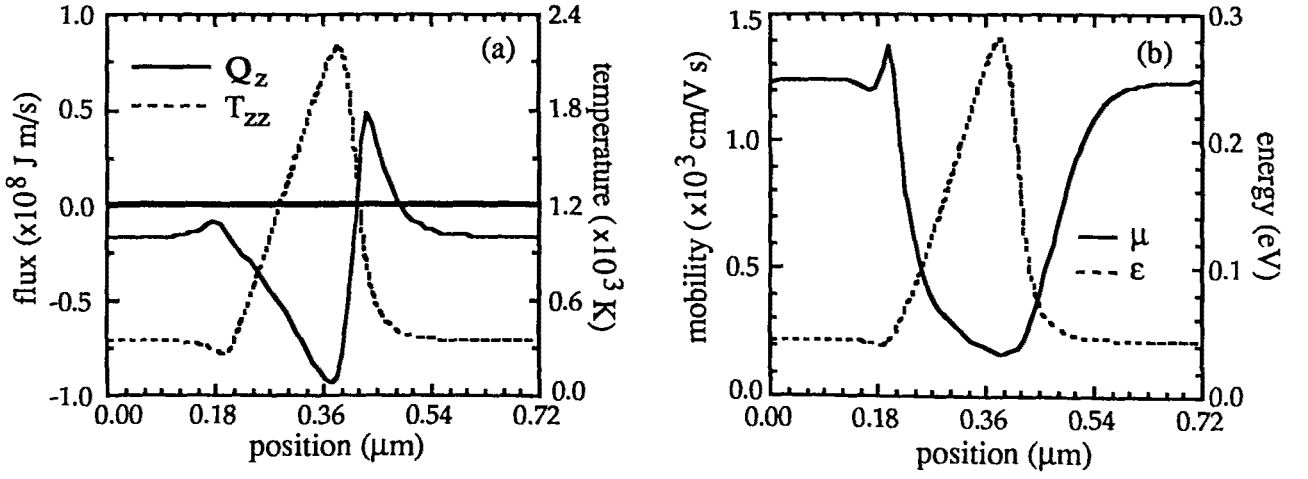

Fig 4. (a) The heat flux (Q_z) and the z diagonal element of the electron temperature tensor (T_{zz}) as computed in the n-i-n (the right boundary has been extended from the previous plots). Note that Fourier's law ($Q_z = -k\nabla T$) is violated both in the bulk regions and where the field decreases rapidly. (b) The carrier mobility (μ) and energy (ε) in the same device. Notice mobility is not a single valued function of the energy.