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Self-consistent Solution of the Boltzmann Transport Equation using the Scattering Matrix Approach

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Abstract

The scattering matrix approach is a new technique for solving the Boltzmann Transport Equation in devices. In this paper, the first self-consistent form of the technique is introduced and demonstrated on an nin diode. Simulation shows that the new technique is computationally efficient and gives accurate, statistically smooth results, making it a promising alternative to Monte Carlo analysis.

As device dimensions continue to shrink, non-equilibrium effects are becoming more important and the need for improved techniques to simulate them is increasing. The Monte Carlo method [1] is an accurate technique for simulating such effects but suffers from high computational demands and other difficulties related to its statistical nature. A new simulation technique, the Scattering Matrix Approach (SMA), has recently been introduced which has an accuracy comparable to Monte Carlo with less computational burden and statistical problems. Typical SMA simulations using pre-computed scattering matrices take only a few percent of the CPU time required for Monte Carlo analysis and exhibit far less statistical noise. In addition, the modularity of the technique holds promise for hybrid simulation of devices involving classical, semi-classical, and even quantum mechanical transport descriptions.

Previous work has demonstrated the SMA to be an efficient, accurate method for simulating high field transport [2] and for simulating transport through low-field and barrier regions [3]. This paper extends this work by reporting the first self-consistent calculations. The results of self-consistent simulation of an nin diode show that the potential converges to a smaller residual than for Monte Carlo analysis of the same structure, while the computational efficiency of the SMA is shown to be at least two orders of magnitude faster.

The Approach

The SMA is an extension of the flux method introduced by McKelvey in 1961 [4]. In the SMA, the device is viewed as a set of interconnected thin slabs, as shown in Figure 1, circles 1 and 2. Each slab is thin enough such that the electric field and doping can be considered constant within it. Transport across each slab is described by a scattering matrix which relates the incident carrier fluxes to the emerging fluxes through transmission and reflection coefficients. In order to model the correct velocity distribution, the carrier flux is discretized into a finite number of subfluxes, or modes, in momentum

space. Thus, the transmission and reflection coefficients in the scattering matrix become matrices themselves relating all the individual incoming and outgoing modes (Figure 1, circle 3). The discretization of the flux is necessary to describe semi-classical transport and represents a departure from the method of McKelvey, who used only one mode scattering matrices.

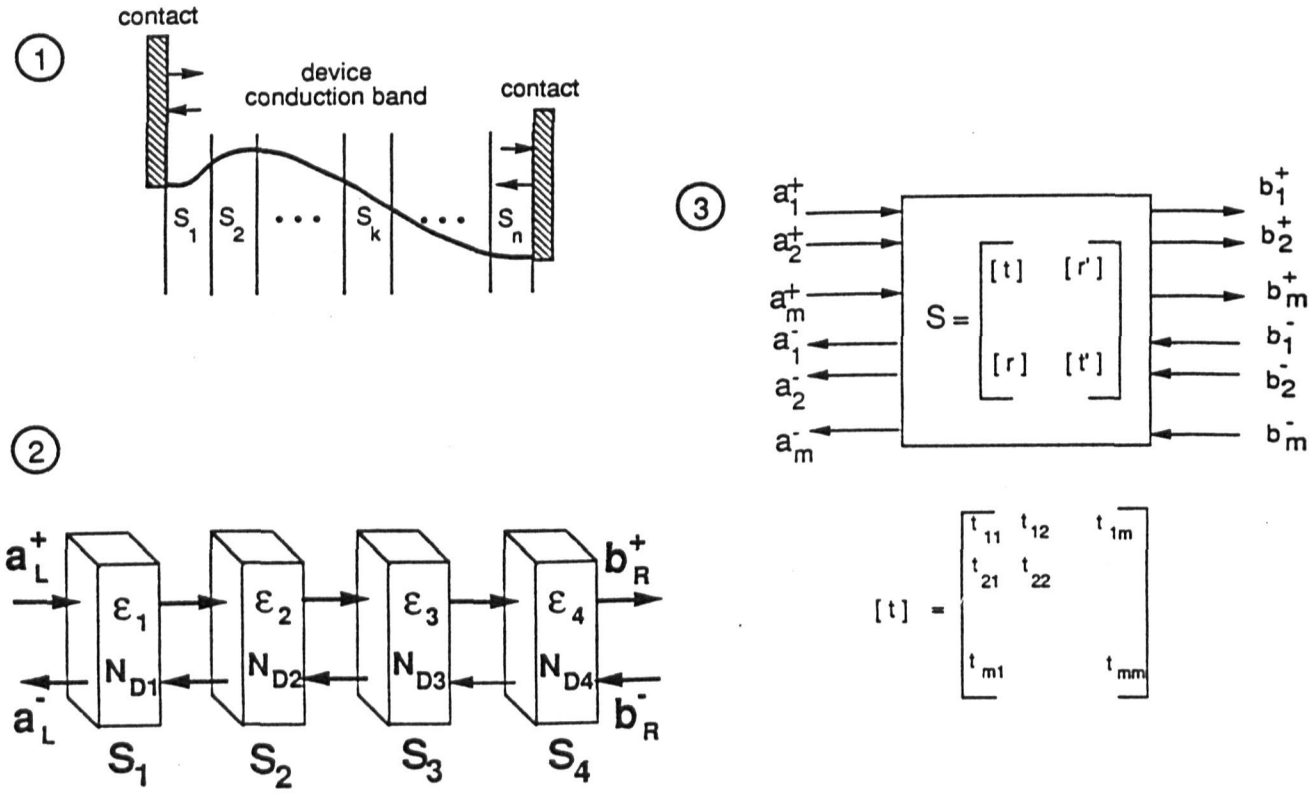

Figure 1 Basic concepts of the scattering matrix approach to device simulation. The device is divided into slabs (1), which are represented by scattering matrices (2), which model transport of a number of carrier fluxes or modes in momentum space (3).

For this work, the scattering matrices were generated by Monte Carlo analysis of bulk slabs under constant fields using a realistic bandstructure [5]. Scattering from ionized impurities was not included. The number of modes employed was 100 and the width of each slab was 98 Å. Scattering matrices were computed for 10 different fields values, ranging from 0 V/cm to the maximum field expected to occur in the device, and then stored in a library. The elements of the matrices were generated by injecting electrons with momenta from a given mode and keeping track of the modes the electrons exited by. Note that these scattering matrices are quite accurate because the thin slabs allow for efficient Monte Carlo simulation of hundreds of thousands of electrons.

The device itself was divided into 60 slabs, and the scattering matrix for each slab was interpolated from those in the library according to the electric field within the slab. The ability to obtain an accurate scattering matrix for an

arbitrary field by linearly interpolating the elements of scattering matrices with adjacent fields was demonstrated in [2]. The scattering matrices were then cascaded together and known fluxes injected from the contacts. The fluxes throughout the device were evaluated using a simple iterative procedure. In order to save computation time, the convergence criteria for the electron concentration in these iterations was made only as strict as necessary for the self-consistent potential to continue to converge. From the fluxes, the distribution function and other quantities of interest were computed.

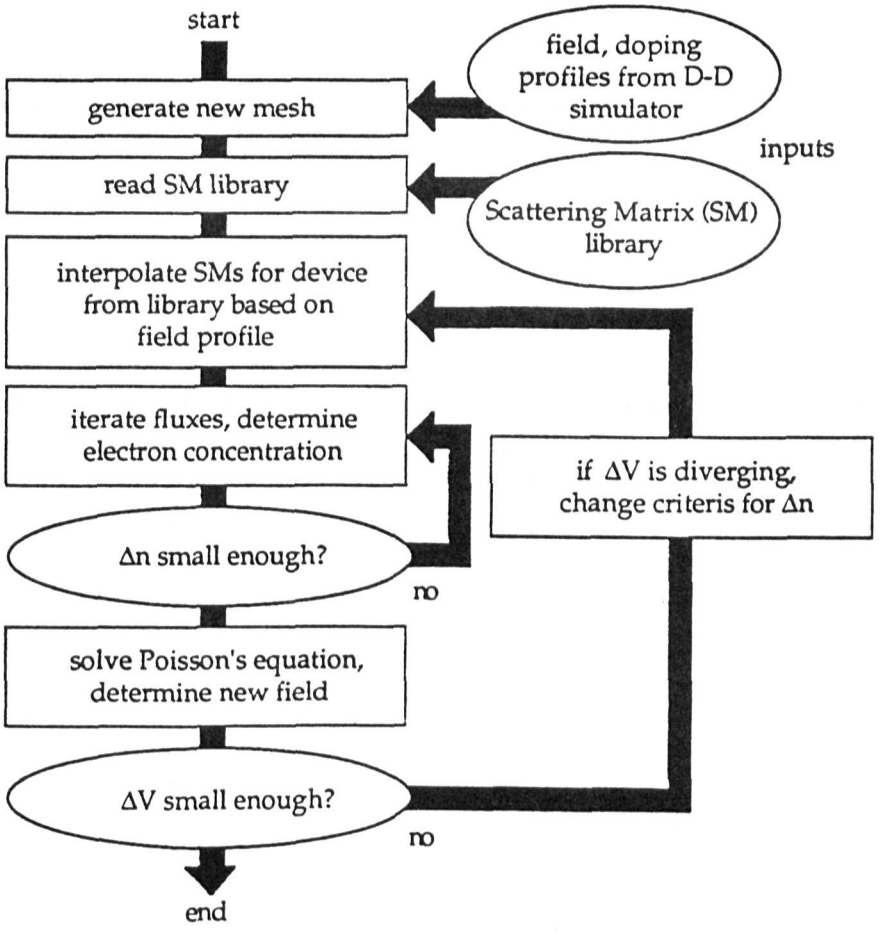

Figure 2 Flowchart detailing the self-consistent SMA to device simulation.

To obtain self-consistency, the process described in the above paragraph is iterated as illustrated in the flowchart of Figure 2. Each time the fluxes through the device were evaluated, the carrier concentration versus position was determined and Poisson's equation was solved to update the electric field. New scattering matrices were then interpolated for each of the 60 slabs in the device from matrices in the original library, and the procedure continued until the potential converged. Note that Monte Carlo analysis was used only to compute the original matrix library; however, during the simulation of the device this library was used repeatedly to interpolate new scattering matrices for every slab in the device each time the field was updated.

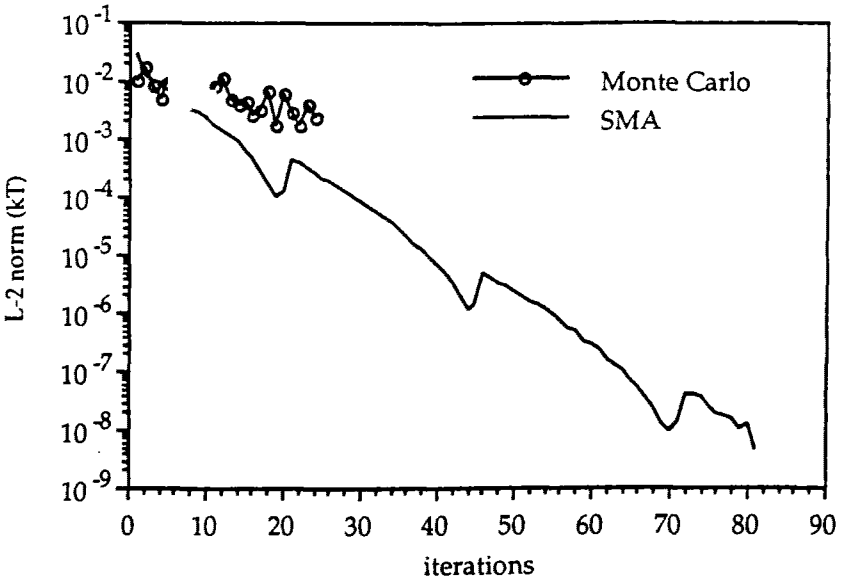

Figure 3 Normalized L-2 norm vs. iteration for SMA and Monte Carlo nin diode simulation.

Results

To demonstrate the self-consistent SMA, a Si nin diode was simulated using the potential from a drift-diffusion simulator as an initial guess. The device consisted of a 0.40 μm layer doped 2×10^{15} cm^{-3} between two 0.08 μm layers doped 5×10^{17} cm^{-3} and was biased 1.5 volts. The convergence behavior is displayed in Figure 3, which shows the normalized L-2 norm for the potential corrections (the euclidean length of the error vector) versus iteration (number of times Poisson's equation is solved). The continuous line is from SMA simulations using $\Delta V_{max} < 10^{-7}$ kT between successive iterations as the convergence criteria for the potential. The discontinuities result from making the convergence criteria for the electron concentration stricter when necessary in order to allow the potential to continue to converge. Though increasing the number of iterations, overall computation time using this method is greatly reduced because, on average, less calculation is required to evaluate the fluxes each iteration. The line with circles is from direct self-consistent Monte Carlo simulation of the same device. Each circle roughly represents a simulation of 6000 electrons, though substantially more electrons are used in the higher numbered iterations.

Comparison of the two results reveals that the SMA can attain a much tighter convergence criteria, comparable to that of drift-diffusion simulators. The L-2 norm computed by the SMA is less than 10^{-8} kT at the final iteration while the Monte Carlo values tend to fluctuate around the 10^{-3} kT range after 15 iterations, a result representative of self-consistent Monte Carlo programs [6]. In addition, the entire SMA simulation, all 81 iterations, was performed in approximately one third the time needed by the Monte Carlo program to complete just one iteration. Thus, for the nin simulation the SMA is over 200 times faster per iteration than Monte Carlo analysis. The one concession

of the SMA to Monte Carlo simulation is that it required approximately 10 times more memory.

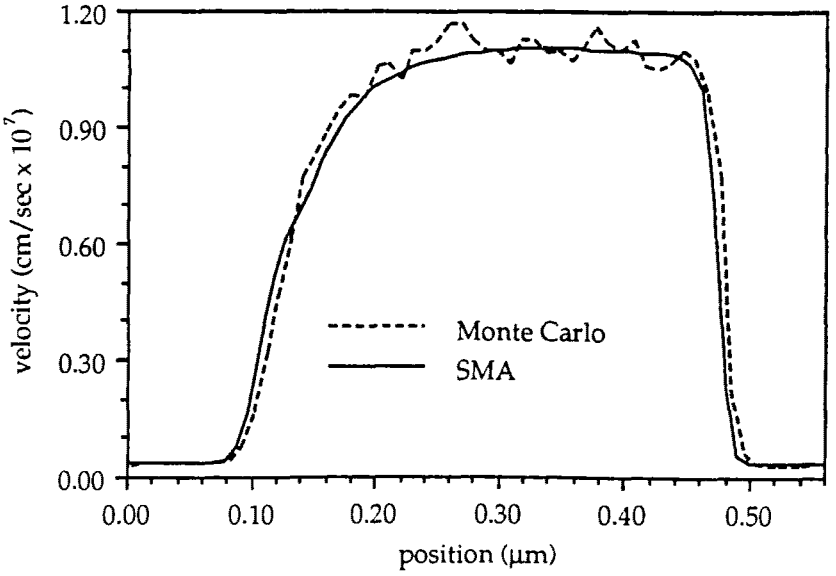

Figure 4 Average electron velocity vs. position in the nin diode.

The reason for the improved convergence can be seen in Figures 4 and 5, which show both the SMA (solid line) and Monte Carlo (broken line) results for the velocity and energy vs. position in the nin diode. The velocity characteristic computed by the SMA is much smoother and lies near the mean of the Monte Carlo values. The SMA result for the energy also exhibits less noise; however, it slightly overestimates the energy given by Monte Carlo. This discrepancy is a result of discretization error caused by using only 100 modes to discretize the fluxes. The accuracy of the energy, which in general is a more sensitive quantity than velocity, appears to depend strongly on the resolution of the distribution function. A more correct energy characteristic can be obtained by increasing the number of modes or possibly by rearranging the modes in energy space. The mild misalignment of the characteristics given by the SMA and Monte Carlo is due to the slightly different fields present in the final iterations of the respective simulations.

Like Monte Carlo, the SMA solves directly for the distribution function which is shown in Figure 6 for several positions in the device and plotted against the electric field of the final iteration. The plot shows the expected spreading of the distribution function as the electrons are heated from the high field region while going from the left to the right contact. The slightly coarse look is due to only using 100 mode resolution to discretize the fluxes. Better resolution can be obtained at the expense of greater memory requirement.

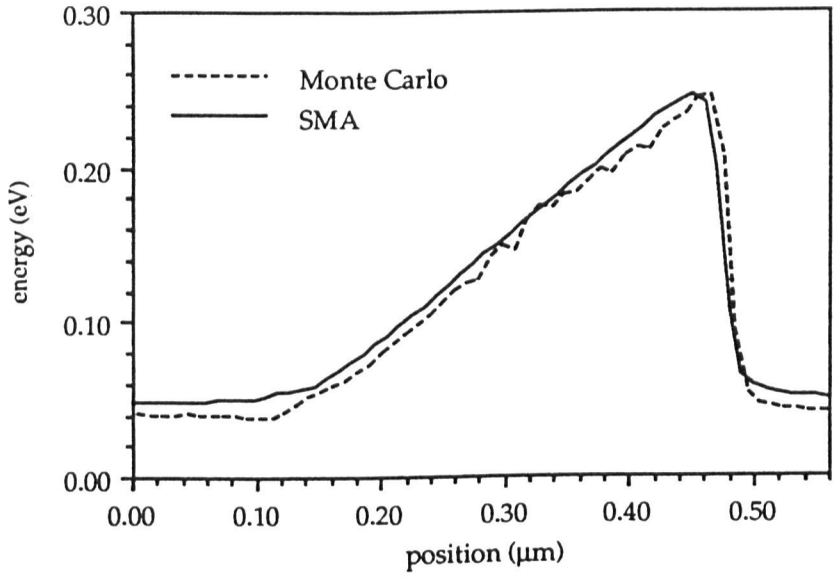

Figure 5 Average carrier kinetic energy vs. position in the nin diode.

Summary

The scattering matrix approach is a new technique for solving the Boltzmann Transport Equation under off-equilibrium and spatially non-uniform conditions. In this paper, the first self-consistent calculations using the SMA were reported. The results for the potential of an nin diode were shown to converge to a residual almost five orders of magnitude smaller than possible by Monte Carlo simulation and at least two orders of magnitude per iteration faster. Monte Carlo results were reproduced without the statistical noise typically associated with the Monte Carlo method. The reduced CPU time and statistical noise along with the ability to accurately simulate both low field and barrier regions, typical problem areas for Monte Carlo analysis, make the SMA a promising technique for simulating advanced devices.

Acknowledgement

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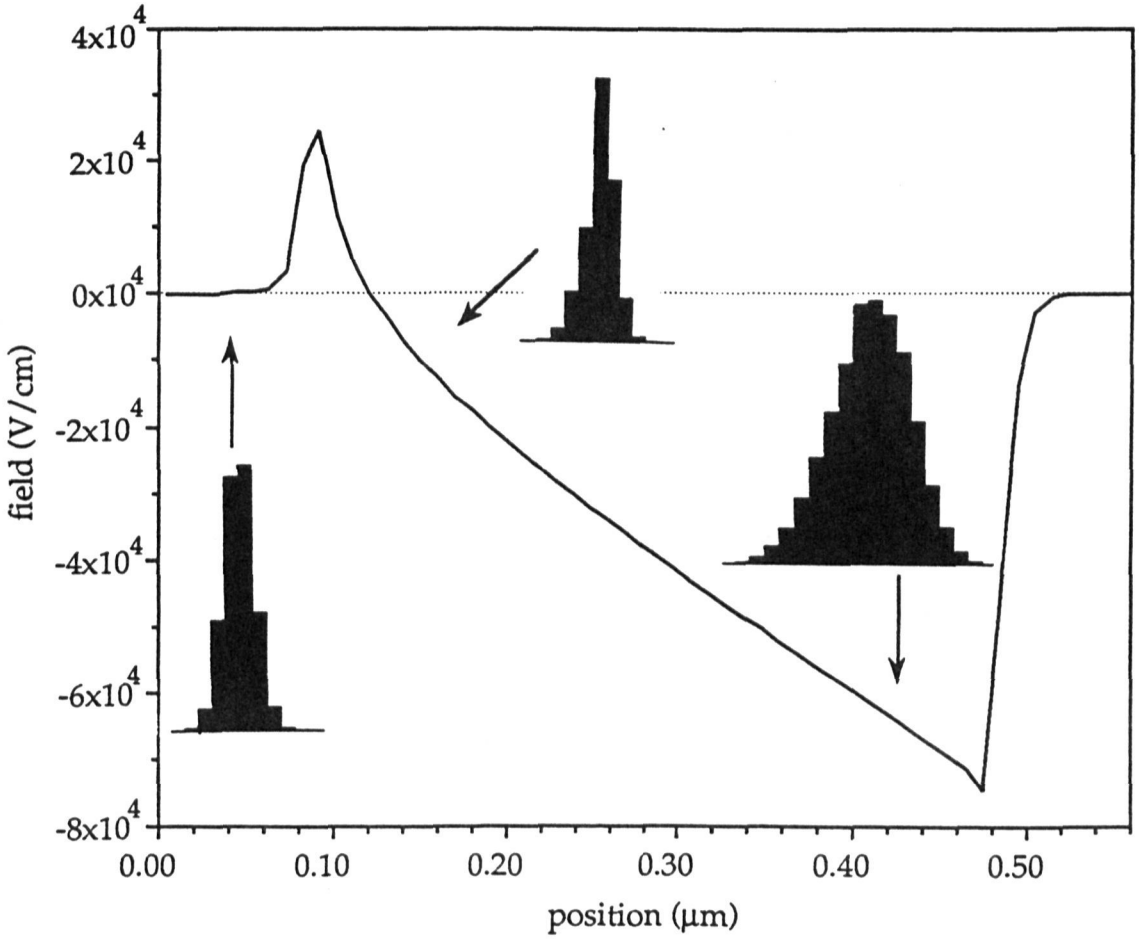

Figure 6 Velocity histograms at various positions in the nin diode (plotted against the field).

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