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# Self-consistent scattering matrix calculation of the distribution function in semiconductor devices

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The scattering matrix approach is a new technique for solving the Boltzmann equation in devices. We report a self-consistent application of the technique to realistic silicon devices exhibiting strong nonlocal effects. Simulation of a hot-electron, *n-i-n* diode demonstrates that the new technique efficiently and accurately reproduces Monte Carlo results without the statistical noise, allowing much tighter convergence with Poisson's equation.

Aggressive downscaling of device dimensions and the use of heterojunctions is increasing the role of nonequilibrium transport in devices. Monte Carlo (MC) simulation[1] is a rigorous technique for simulating such effects but suffers from high computational demands and difficulties related to its statistical nature. Hydrodynamic equations can also be used, but the numerous simplifying approximations employed in their derivation can lead to nonphysical results when simulating devices. These difficulties have sparked interest both in developing methods to extend the capabilities of conventional MC[2] and in creating other techniques to directly integrate the Boltzmann equation.[3] One of these latter techniques, the scattering matrix approach (SMA), has demonstrated an accuracy comparable to MC while giving virtually noise-free results at significantly reduced computational requirements.[4] Previous SMA work involved non-self-consistent simulation of model structures with piecewise constant electric fields.[4] In this letter we demonstrate the first self-consistent scattering matrix simulations of realistic silicon devices displaying strong velocity overshoot.

In the SMA, the device is viewed as a set of interconnected slabs, with each slab sufficiently thin so that the doping and electric field can be considered constant within it. As shown in Fig. 1, 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; since we are concerned with semiclassical transport, these coefficients are real numbers between 0 and 1. In order to resolve the velocity distribution, the flux is discretized into $M$ finite bins in momentum space called modes. The elements of the $2M \times 2M$ scattering matrices are then computed by MC 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.[4]

For the simulation results given here, momentum space was uniformly discretized from 0 to 2.5 eV into 20 longitudinal and 20 transverse modes (modes with momenta parallel and perpendicular to the field, respectively), for a total of 400 modes. Using a MC program based on the work of Reggiani and Jacoboni,[1] scattering matrices were then calculated for 100-Å-wide, ⟨111⟩-oriented silicon slabs at 11 different fields, ranging from 0 to $2 \times 10^5$ V/cm. Within each slab, 20 000 electrons were injected into each mode with longitudinal momenta distributed across the mode according to $\exp(-p_z^2/2m^*kT_e)$, where $p_z$ is the longitudinal momentum within the mode, $m^*$ is the energy-dependent effective mass, and $T_e$ is the field-dependent electron temperature as determined from bulk MC simulations. This distribution gives more accurate results than the uniform distribution used in Ref. 4.

To solve for the distribution function in a device self-consistently, an initial estimate for the electric field profile is first established by performing a drift-diffusion simulation of the structure. The device is then divided into 100-Å-wide slabs and scattering matrices for each slab are evaluated by interpolating matrices in the precomputed library according to the field within the slab. The scattering matrices are then cascaded together and fluxes are injected at the two contacts. The injected fluxes are assigned the same distributions in momentum space as those in a bulk semiconductor with the same electric field as found near the contacts (thus effectively treating the contacts as infinite bulk regions). The fluxes throughout the device are evaluated using a simple iterative technique for cascading scattering matrices.[4]

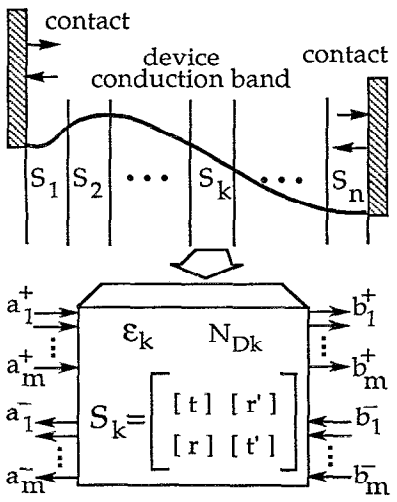


FIG. 1. Basic concept of device simulation in the SMA. The device is divided into slabs which are each represented by a scattering matrix, $S_k$. Each matrix models the transport of a number of carrier fluxes resolved in momentum space through the slab. The coefficients of $S_k(t,t',r,$ and $r')$ are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



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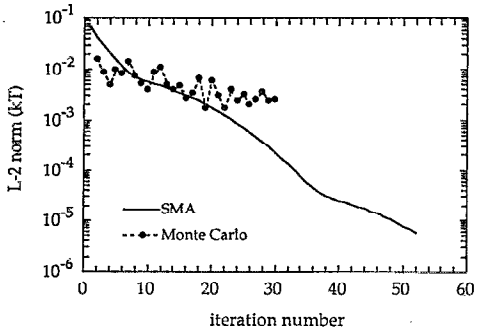


FIG. 2. Normalized $L$-2 norm vs iteration for SMA and Monte Carlo $n^+$-$n$-$n^+$ diode simulations.

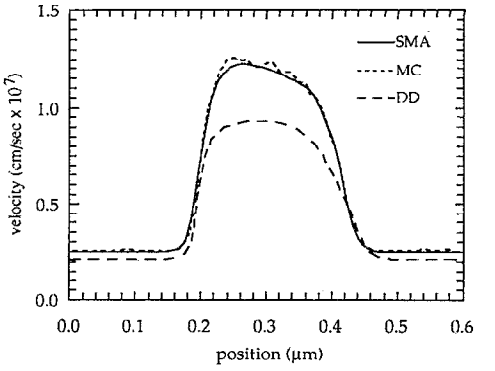


FIG. 3. Average electron velocity vs position in the $n^+$-$n$-$n^+$ diode as computed by SMA, Monte Carlo (MC), and drift-diffusion (DD) analysis.

From the fluxes, the steady-state electron concentration, velocity, energy, and distribution function between each slab are computed. The contacts are then checked for space-charge neutrality; since the boundary conditions specify only half of the flux (the incident flux), the electron concentration at the contact may not equal the doping after the fluxes are evaluated. If space-charge neutrality is violated, the injected flux is scaled to give the correct concentration and the above procedure (with the exception of interpolating the scattering matrices) is repeated until neutrality is achieved. Next, Poisson's equation is solved to update the electric field. Based on this new field profile, new scattering matrices are then interpolated for each slab in the device using the original library, and the entire simulation procedure repeats until the potential converges. Note that MC analysis is used only to compute the original matrix library; during the simulation of the device this library is used repeatedly to update the scattering matrices. When the transmission and reflection coefficients of the scattering matrices are evaluated by semiclassical techniques, the SMA can be shown to be a rigorous solution to the spatially inhomogeneous Boltzmann equation.

To demonstrate the application of the SMA to self-consistent device simulation, we present results for a highly based Si $n^+$-$n$-$n^+$ diode. The device consists of a 0.20-$\mu$m layer doped $2\times10^5$ cm$^{-3}$ between two 0.20-$\mu$m layers doped $5\times10^{17}$ cm$^{-3}$ and was biased 1.5 V. The device was divided into 60 100-Å slabs, each represented by a scattering matrix. The convergence behavior of the potential, represented by 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) is shown in Fig. 2. In this figure, the solid line is from SMA simulations using $\Delta V_{\max} < 10^{-5}$ kT between successive iterations as the convergence criterion for the potential, while the line with circles is from direct self-consistent MC simulation of a similar structure. Comparison of the two results reveals that the SMA is able to obtain tighter convergence, comparable to that of drift-diffusion simulators. At the final iteration, the $L$-2 norm computed by the SMA is less than $10^{-5}$ kT while the MC values tend to fluctuate above $10^{-3}$ kT after approximately 20 iterations, a result typical for most self-consistent MC programs.[5]

The reason for the improved convergence can be seen in Figs. 3 and 4, which compare the results given by the SMA (solid line), MC (dotted line), and the drift-diffusion method (dashed line) for the velocity and energy versus position in the $n^+$-$n$-$n^+$ diode. In order to make a more consistent comparison, the MC simulation for these results was performed using the final field determined in the SMA solution. Both SMA and MC results exhibit significant velocity overshoot in the high-field region (the saturation velocity in Si is $1.0\times10^7$ cm/s), an effect unresolved by the classical drift-diffusion equations with a field-dependent mobility. Velocity overshoot increases the current, thus the SMA and MC results show higher velocities in the contact regions than the drift-diffusion results. The velocity characteristic computed by the SMA, however, is much smoother than the MC result, which contributes to its improved convergence behavior. The SMA result for the energy also exhibits less noise and shows good agreement with MC simulation at both low and high fields, the difference being less than 5%. These results show an improvement over the characteristics given in Ref. 4 due to the more realistic injection conditions used when generating the scattering matrices. The slightly greater disparity between the MC and SMA results in the high-field region originates from discretization error caused by resolving momentum space into finite-sized bins. This error can be reduced by using a greater number of modes to resolve the distribution function.

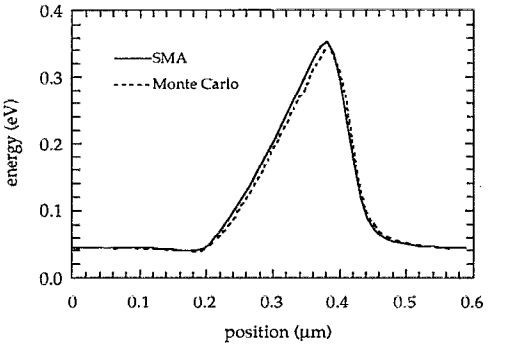


FIG. 4. Average kinetic energy vs position in the $n^+$-$n$-$n^+$ diode.

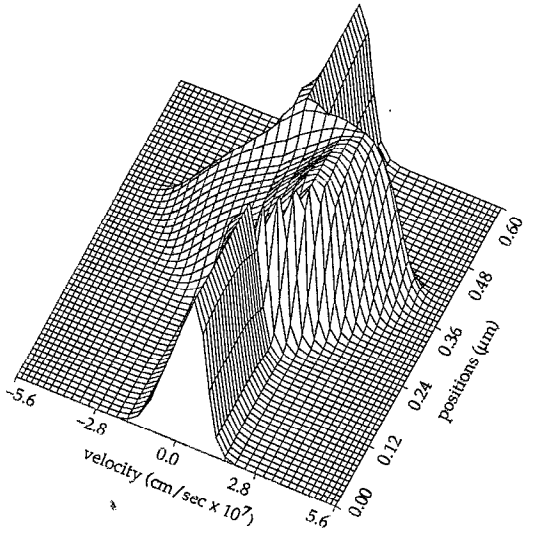


FIG. 5. Normalized distribution function of the longitudinal electron momentum throughout the diode.

Since the SMA treats semiclassical transport rigorously, it resolves the carrier distribution function throughout the device. Figure 5 shows the normalized distribution function for the longitudinal momentum taken along cross sections of the device. In the cathode, the distribution function is Maxwellian, slightly shifted because current is flowing. In the high-field region, the distribution becomes heated and rapidly displaced, displaying a long, highly non-Maxwellian tail of populated negative momentum states. Near the anode the distribution again returns to a Maxwellian shape as the distribution cools in the low-field region. The slightly coarse look is due to using only 20 modes to resolve longitudinal momentum space.

In conclusion, the scattering matrix approach is a new technique for solving the Boltzmann equation under strongly off-equilibrium and spatially nonuniform conditions. In this letter, the first self-consistent calculations using the SMA in devices dominated by highly nonlocal effects were reported. Simulation of a highly biased $n^+$-$n$-$n^+$ diode show that Monte Carlo results were reproduced without statistical noise, allowing the fluctuations in potential to converge to a value at least three orders of magnitude smaller than possible by the Monte Carlo technique. The statistically smooth results along with the ability to treat problems that are difficult for Monte Carlo simulation (e.g., low-field regions, barriers, recombination-generation) make the SMA an excellent technique for simulating advanced devices.

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