FULL BAND S-MATRIX SIMULATION OF ELECTRON TRANSPORT IN SI

Carl Huster and Mark Lundstrom
1285 Electrical Engineering, Purdue University, W. Lafayette, IN 47907
(317) 494-3372 huster@ecn.purdue.edu lundstro@ecn.purdue.edu

Abstract

The scattering matrix approach to device simulation is extended to include the full bandstructure of silicon as evaluated by the emperical psuedopotential method. Both a determinsitic and a fast stochastic solution technique are presented. Results are given for bulk silicon and for a non self-consistent structure. Descretization of the Brillouin Zone is idetified as an key issue. It is concluded that one dimensional full band simulations are feasible on contemporary workstations.

I. Introduction to the Scattering Matrix Approach

The scattering matrix approach (SMA) is a deterministic technique for solving the Boltzmann Transport Equation. The problem is set by dividing the device into thin slabs and resolving the carrier fluxes between them into modes in momentum space as shown in fig. 1. The thickness of the slabs is typically 10 to 100A and need not be uniform throughout the device. The maximum slab thickness in a particular region of the device is determined by the spatial resolution requested by the user or the maximum allowable potential drop across a slab. Transport across each slab is treated by a scattering matrix. A column of a scattering matrix relates an incident mode in momentum space to all exiting modes in momentum space. The scattering matrices are generated by a Monte Carlo experiment. A number of carriers in a particular incident mode in momentum space are shot at thin slab of semiconductor. The exiting distribution of them in momentum space is mapped onto a column of the scattering matrix.

A self-consistent solution is achieved by a three step iterative process. First, the scattering matrices appropriate for the electric fields throughout the device are determined. This is done by interpolating between matrices in a library. Second the electron and hole fluxes are solved for. Thirdly the new potential distribution is determined by solving Poisson's equation for the new charge distribution. These steps are repeated until convergence has been achieved.

Presently we have two techniques available for solving for the fluxes. The first is a deterministic technique using Gauss-Seidel iterations. It operates by sweeping from left to right through the device and back. At each slab the exiting fluxes are updated based on the current guess at the incoming fluxes. One cycle through the device is a Gauss-Seidel iteration. It should be pointed out that Gauss-Seidel techniques are known to converge slowly and that accèleration techniques do exist. The second technique is a stochastic technique that we refer to as scattering matrix Monte Carlo. In the field of neutron transport the same idea is referred to as condensed history Monte Carlo. The technique operates by following a single flux through the device. Instead of the incoming flux being split to all coupled exiting modes, one is selected at random by treating the column of the scattering matrix as a probability distribution. The flux is then transmitted or reflected to the appropriate mode. The advantage of this technique is that it is extremely fast compared to the deterministic technique. The disadvantage is that statistical noise is present in a solution generated this way.

II. Full Band Work

We consider the full band work done to date to be a feasibility study. The work has focused on the issues of how to discretize the Brillouin Zone and how to deal with the large sparse matrices that result. The problem of discretization actually has two parts. First, due to the symmetry of the Brillouin Zone, only a fraction of it must be discretized. In the case of Monte Carlo simulations this fraction is typically 1/48th. For the SMA, the fraction that must be discretized is larger and depends on the real space geometry, crystal orientation, and electric field direction. If the electric field and the transport direction are both along the same <100> direction then 1/8th of the Brillouin Zone must be discretized (fig. 2). If they lie in the same <111> direction then 1/6th of the zone is required. It should be noted though that the first two conduction bands of silicon are treated, so the required fraction of the zone must be discretized twice, once for each band.

The second part of the discretization problem is how to discretize the required portion of the Brillouin Zone. This does not have such a clear cut solution. For the proof of concept work we have used a straightforward cubic discretization in the components of the wave vector. 7413 cubes were used to discretize the irreducible 1/48th of the Brillouin Zone. From using this discretization we have learned that there are problems with it. Since the quantities of interest are the energy and velocity of the carriers, a discretization in the wavevector is not well suited to resolving these quantities. Second, since a mode boundary cannot appear at a constant energy, it is difficult to get the band to band transitions resolved correctly. We are currently investigating other discretization schemes, but the current work is sufficient to establish the viability of the full band S-matrix simulation.

The discretization in the components of the wavevector mentioned above results in very large sparse matrices. Our matricies are generated using the full band Monte Carlo code from the University of Illinois at Urbana Champaign [4]. A typical matrix is approximately 93000 elements on a side, 0.015% full and requires approximately 15MB of storage. A simple extrapolation significantly overestimates the memory requirements for a device simulation due to the existence of a memory saving technique known as splitting. With this and some other techniques in place, the memory requirements for a 1-D device simulations should be only about 35 MB.

III. Results

Thus far two types of simulations have been demonstrated using the full band matrices. The first is of bulk silicon with an electric field applied. Due to its speed and simplicity this is usually the first test of a new scattering matrix. The simulation is done by imposing periodic boundary conditions on a single slab or matrix and iterating until convergence is achieved. The periodic boundary conditions are equivalent to and infinite chain of such slabs. Results are presented here for electric fields of 300kV/cm (fig. 3) and 1kV/cm (fig. 4). Notice that at 300kV/cm both the SMA and the scattering matrix Monte Carlo closely match the direct Monte Carlo results. This is expected since the scattering matrices were generated with the same Monte Carlo program that produced the results. Notice however that the deterministic solution technique (SMA) resolves the distribution accurately for several orders of magnitude beyond the stochastic techniques (direct Monte Carlo and scattering matrix Monte Carlo). At 1kV/cm the results do not match so well due to the poor discretization at low energies and the problems it has with coupling to the second band.

Results using the SMA and scattering matrix Monte Carlo for a non-self consistent model structure are presented in fig. 5. This structure features three electric field regions of 1kV/cm, 300kV/cm and 1kV/cm with periodic boundary conditions applied. Notice that both the velocity overshoot and undershoot are well resolved. Also notice that the low field saturation velocity is about four times higher than it should be. One factor of two is due to our discretization of momentum space. The other factor of

two is due to the fact that the Monte Carlo program was designed for studying high field transport and does not accurately reproduce low field results. There are two primary differences between the two results. First, since the scattering matrix Monte Carlo technique is stochastic, it shows statistical noise. Second, the scattering matrix Monte Carlo takes 57 seconds to run on an RS6000/580 while the SMA takes 2500 seconds using a Gauss-Seidel iteration accelerated by a technique known as fine mesh rebalancing.

IV. Conclusions

We have four important conclusions about the full band scattering matrix approach. First, the results presented here demonstrate that one dimensional full band self consistent simulations are feasible on contemporary workstations. Second, discretization of the Brillouin Zone is a key issue that must be addressed. Third, the scattering matrix Monte Carlo technique offers a very fast way of doing Monte Carlo simulations. Finally, the results suggest that two dimensional full band simulations should be feasible on high end workstations or parallel computers.

[1] A. Das and M. S. Lundstrom, "A Scattering Matrix Approach to Device Analysis," *Solid-State Electron.*, Vol. 33, pp. 1299-1307, 1990.

[2] M.A. Alam, M. A. Stettler, and M. S. Lundstrom, "Formulation of the Boltzmann Equation in Terms of Scattering Matrices", *Solid-State Electronics,* Vol. 36, pp. 263-271, 1993.

[3] M. A. Stettler and M. S. Lundstrom, "Self-consistent scattering matrix calculation of the distribution function in semiconductor devices.," *Appl. Phys. Lett.,* Vol. 60, pp. 2908-2910, 1992.

[4] K. Hess, ed., *Monte Carlo Device Simulation: Full Band and Beyond,* Kluwer Academic, Boston (1991).

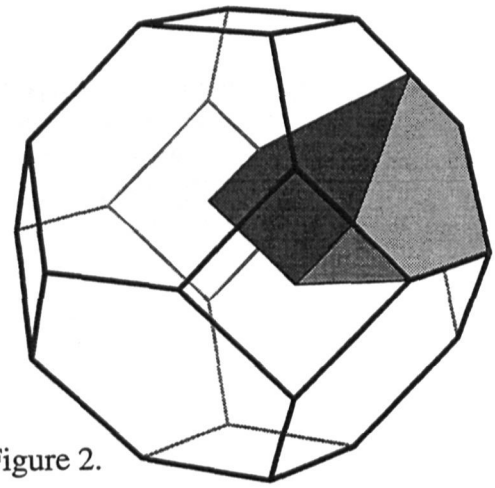
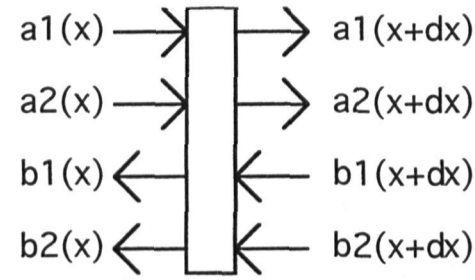


Figure 2.



$$\begin{bmatrix} a1(x+dx) \\ a2(x+dx) \\ b1(x) \\ b2(x) \end{bmatrix} = \begin{bmatrix} t11 & t21 & r'11 & r'21 \\ t21 & t22 & r'21 & r'22 \\ r11 & r21 & t'11 & t'21 \\ r21 & r22 & t'21 & t'22 \end{bmatrix} \begin{bmatrix} a1(x) \\ a2(x) \\ b1(x+dx) \\ b2(x+dx) \end{bmatrix}$$

Figure 1.

Fig. 1 Section of the Brillouin zone discretised for one-dimensional transport simulation. The electric field is assumed to lie along a <100> direction. Symmetry considerations dictate that 1/8th of the BZ, or 6 irreducible wedges are needed.

Fig. 2 Definition of fluxes and the full band scattering matrix. Subscripts refer to the band, 1 or 2, and each flux is an M X 1 vector, where M=22239.

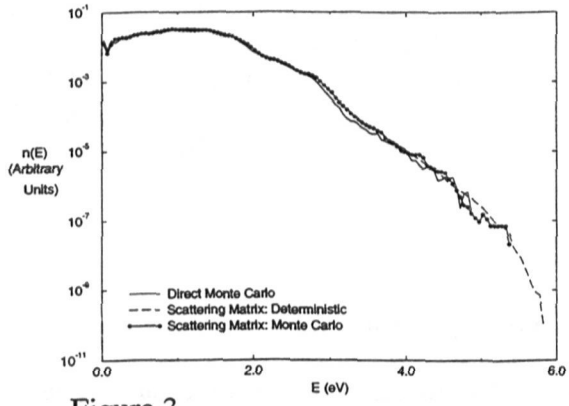


Figure 3.

Fig. 3 Computed energy distributions for electrons in bulk Si at an electric field of 300kV/cm. For comparison, we also display the results of a direct Monte Carlo simulation using the same program used to evaluate the S-matricies [4]. For the S-matrix approach, we show results for a deterministic solution procedure as well as for Monte Carlo solution procedure.

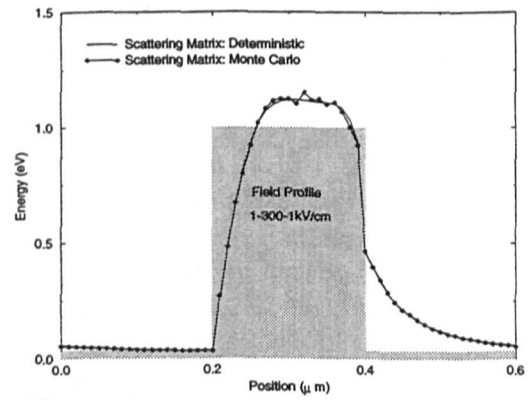
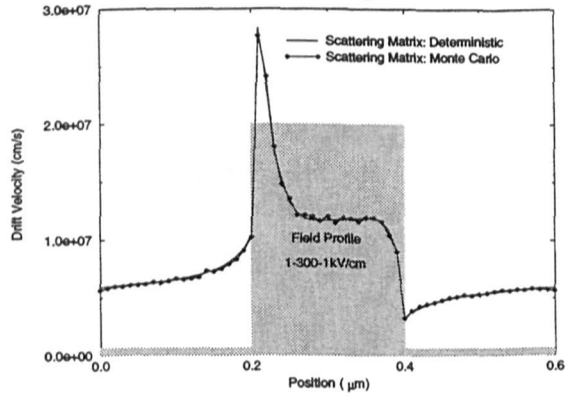


Figure 4.

Figure 5.



Figs. 4&5 Computed average energy and velocity vs. position for electron transport in a model Si device consisting of a low-high-low field profile. Again, results are shown for both the deterministic and Monte Carlo solution techniques. The Monte Carlo S-matrix solution took 57sec on an IBM RS-6000/580 workstation, most of which was overhead involving loading of the matricies.