Memory Efficient Scattering Matrix Device Simulation by Decomposing the Effect of Carrier Scattering and Field Acceleration

Mark A. Stettler, Muhammad A. Alam, and Mark S. Lundstrom
School of Electrical Engineering, Purdue University, West Lafayette, IN 47907 USA

Solving the Boltzmann equation (BE) has typically been a trade-off between memory and speed. Monte Carlo simulation is generally slow but memory efficient, while deterministic techniques are faster but significantly more memory intensive. The Scattering Matrix Approach (SMA) [1-3] belongs to this latter class of BE solutions and thus has also suffered from extensive memory requirements. These requirements, however, have now been substantially reduced by introducing a new technique to decompose the effects of scattering and the electric field on carrier transport. This reduction makes even detailed multi-band and 2-D device simulation feasible on today's modestly equipped workstations.

The technique of separating carrier scattering from field acceleration, which can be mathematically justified for a thin slab, is shown in Fig. 1. In the SMA, the device is divided into thin slabs which are each represented by a scattering matrix. Previously, each scattering matrix characterized both the effects of scattering and the electric field on carriers in discretized momentum space. Many matrices had to be stored because, for a realistic device, the electric field differs for each slab. In the new technique, the field acceleration and the scattering processes are treated by separate matrices. Despite the added number of matrices, the memory requirements are now drastically reduced because only a few symmetrical "scattering process" matrices need to be stored for the entire device and the "field" matrices, which are still needed for every position, are extremely sparse (see Fig. 2). For example, storing all the matrices for a 100 slab device in highly discretized momentum space requires almost 500 MB using the old method, but less than 20 MB after using the decomposition technique. This new technique has been implemented in scattering matrix simulators for both Si and GaAs devices. As shown in Fig. 3, the new method reproduces the bulk velocity-field characteristic for single valley electron transport in Si and for three-valley transport in GaAs. Figure 4 shows results for a Si device structure, demonstrating that the decomposition method, which resolves velocity overshoot at the field boundary, is applicable to devices. In our presentation we will discuss recent results such as bipolar and heterostructure device simulation, both of which have been made much more efficient by the decomposition technique.

In conclusion, we have developed a technique that substantially reduces the memory requirements of the Scattering Matrix Approach, a direct solution method to the Boltzmann equation. Using this technique, we will demonstrate memory/computation efficient device simulation involving bipolar and heterostructure transport. An important ramification of this technique is that full-bandstructure and 2D and 3D simulation, previously thought memory prohibitive for direct solutions to the BE, should be feasible even for the capacity of today's workstations.

[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. 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.

[3] M. A. Alam, M. A. Stettler, and M. S. Lundstrom, "Formulation of the Boltzmann equation in terms of scattering matrices," *Solid-State Electron.*, Vol. 36, pp. 263-271, 1992.

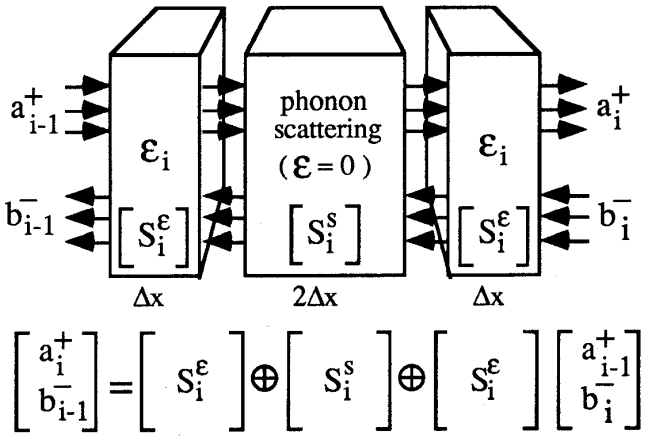

Fig. 1

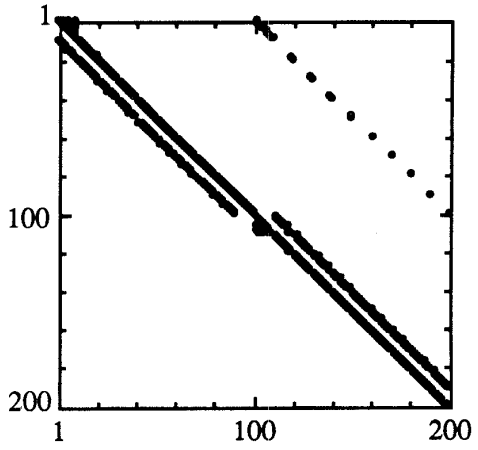

Fig. 2

Fig 1-2. Descretized flux transport through each slab in the device is modeled by three matrices: a matrix with transport coefficients determined only by phonon scattering (no electric field) cascaded between two matrices with coefficients determined only by the electric field (no scattering). To properly weight both effects, the electric field matrices are computed for slabs with half the width of the phonon scattering matrices. Memory savings occur because only a few symmetrical phonon scattering matrices have to be stored for the entire device and the electric field scattering matrices are sparse. Fig. 2 shows a typical electric field matrix using a 100 mode discretization. The dark circles indicate nonzero elements. Note that because ionized impurity scattering scattering is elastic, it also gives rise to sparse matrices and thus can be treated in a manner similar to the electric field.

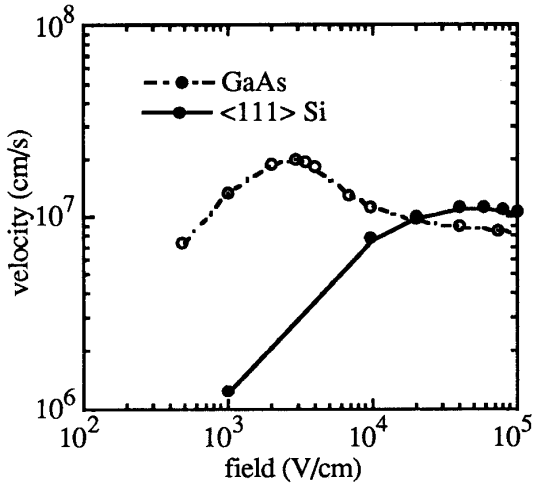

Fig. 3

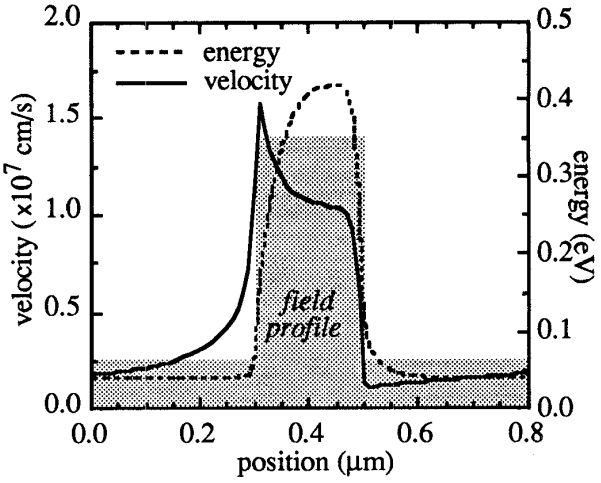

Fig. 4

Fig.3-4. GaAs and Si velocity field curves computed using the above method. Fig. 4 shows results for a model Si device structure (field is -10^3, -10^5, -10^3 V/cm respectively). Note that velocity overshoot at the field boundary is resolved.