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A Scattering Matrix Approach to Advanced Bipolar Device Simulation

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Abstract- The scattering matrix approach is a new technique for simulating transport in advanced devices. A device is viewed as an interconnected set of thin semiconductor slabs and transport across each slab of semiconductor is characterized by a probability scattering matrix. Individual scattering matrices are then cascaded to derive the overall device characteristics. In this paper, we will describe briefly the scattering matrix approach, apply it to simulate off-equilibrium effects in model semiconductor devices, and demonstrate its potential for advanced bipolar simulation.

1. Introduction

Off-equilibrium transport effects influence the performance of modern devices such as advanced bipolar transistors with thin bases and collectors [1]. For such devices, drift-diffusion equations aren't valid, hydrodynamic, balance equations require many simplifying assumptions, and Monte Carlo simulations are computationally prohibitive. Our objective is to present a new, efficient approach to simulate off-equilibrium transport in modern devices. The new approach is a general technique for solving the Boltzmann equation in devices and has special advantages for bipolar devices because it can readily treat injection across a barrier and carrier recombination.

2. The Scattering Matrix Approach

Figure 1 shows how the scattering matrix approach is applied to simulate devices [2]. We first divide the device into finite number of semiconductor slabs. Individual semiconductor slabs are characterized by their width, doping density, and the electric field. Next, a probability scattering matrix is computed to represent the transport of electron flux through the individual slabs. The scattering matrix connects the incoming fluxes to the slab to the outgoing fluxes through transmission and reflection coefficients. Instead of representing the flux of carriers by an average quantity [3], we resolve fluxes in the velocity space by discretizing the velocity space into a finite number of bins or modes [2]. For example, in Fig. 2, we have divided the velocity space into two bins, so, there are 2 incoming modes from each side of the slabs. The size of the scattering matrix with 2 incident and 2 outgoing modes is 4×4, (Fig. 2). An element of the scattering matrix, t_{12} for example, gives the probability of transmission of flux from mode 2 on the left of the slab to mode 1 at the right of the slab.

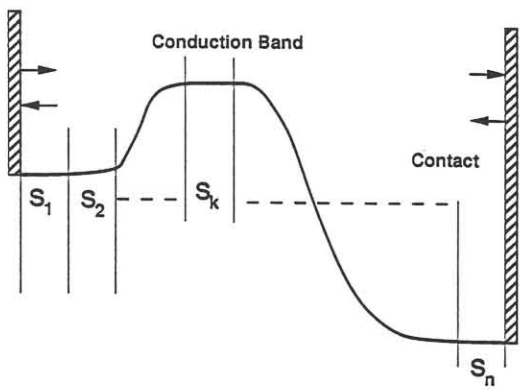

Fig. 1 The figure shows schematically how the scattering matrix approach can be used for device simulation

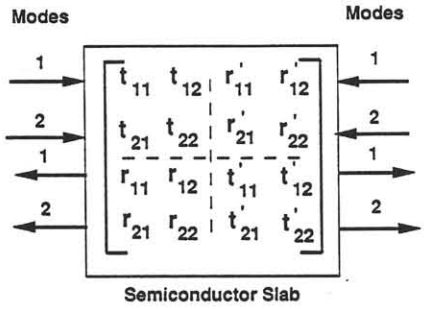

Fig. 2 The figure shows scattering matrix across a slab of semiconductors with 2 incoming and 2 outgoing modes.

By cascading the individual scattering matrices which comprise the device, we can derive important device characteristics such as the average velocity of carriers across the device or the I-V characteristics.

For device simulation application, we might begin with a library of pre-computed scattering matrices for different types of slabs with different values of the electric field. To evaluate the scattering matrix for a thin slab centered at z_i in a device, we would interpolate a scattering matrix for $\mathcal{E}(z_i)$ from the library.

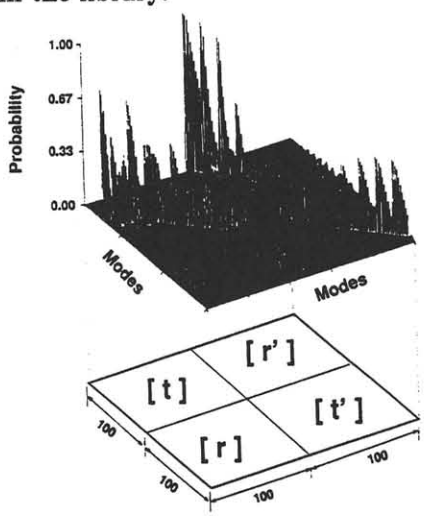

Fig. 3 A sample scattering matrix with 100 modes computed using a Monte Carlo simulator [2].

Scattering matrices can be computed by any technique that can solve the Boltzmann transport equation (BTE) in small uniform slabs of semiconductors. We have used a Monte Carlo simulator to compute the scattering matrices. A sample scattering matrix with 100 modes is shown in Fig. 3. The scattering matrix is for a 98Å wide Si slab with an electric field of 9.0×10^4 v/cm. We compute scattering matrices only once for a given slab, and use the same scattering matrix for more than one device - this results in an enormous savings of CPU time. The elements of the scattering matrix are dependent on the physics of scattering within the semiconductor slab, but not on the boundary condition of the device in which it is embedded.

We verified the accuracy of the scattering matrix approach by simulating bulk average velocity of Si and comparing it to experimentally observed values [2]. We have also shown that interpolated scattering matrix for a value of electric field intermediate between two fields give accurate results [2].

3. Device Simulation

Our goal is to develop the scattering matrix approach into a useful tool for the simulation of advanced devices, such as next-generation Si bipolar transistors. A Monte Carlo simulator has recently been used to simulate bipolar transistors [1], but there are some inherent difficulties associated with the Monte Carlo simulation of a bipolar structure, such as the potential barrier at the emitter-base junction or recombination of carriers. Statistical noise in the computed I-V characteristics is a problem for circuit simulation.

To demonstrate the scattering matrix approach to advanced bipolar simulation, we begin with simple, model device structures which resemble parts of a bipolar transistor. A complete bipolar transistor can be viewed as a combination of accelerating- (collector-base space charge region (SCR)), zero- (such as, quasi-neutral base region), and decelerating-field regions (emitter-base SCR). We first study these three types of regions somewhat independently. Our objectives are: a) to demonstrate the ability of the scattering matrix approach to simulate off-equilibrium effects, such as velocity overshoot, b) to demonstrate that it can treat problems that are difficult for Monte Carlo, and c) to verify the accuracy of the approach.

To demonstrate the ability of the scattering matrix approach to simulate carrier transport along an accelerating field, we have successfully simulated a high-low-high electric field structure using scattering matrices and the results are

presented in [2]. For this example, we have achieved a speed-up by a factor of 20 over Monte Carlo simulation of an identical structure.

Simulating a device under low field is particularly difficult for the Monte Carlo method because of the statistical noise [4]. Statistical noise can be decreased by using more electrons in the Monte Carlo simulation which makes the Monte Carlo method prohibitively CPU time intensive. The scattering matrix approach can handle the noise problem better since we simulate a small slab of semiconductor (100Å), and we can afford to shoot many electrons (we generally shoot 20,000 electrons/mode to compute scattering matrices) to minimize the statistical noise in the scattering matrix. For zero-field scattering matrix, we have the additional advantage that the scattering matrix is symmetric. We need only to shoot from one side of the semiconductor slab.

To simulate bulk Si under zero-field, 20 identical scattering matrices, computed across a 100Å slab under zero field, are combined. The velocity space is resolved into 20×20 (20 modes in the longitudinal velocity space and 20 modes in the transverse velocity space with respect to the direction of the applied electric field) modes. Electrons diffuse through the slab in the absence of an electric field. The zero-field mobility computed from the simulation is approximately 1400 cm^2v/sec which agrees quite well with the experimental observation.

Next, we simulated transport along a decelerating electric field (a barrier). The model device in this case is a metal semiconductor (M-S) diode. Carriers which are initially at high energy can only transmit over a barrier, so, we need to resolve accurately carriers over a wider range of energy than in the case of an accelerating electric field. Potential barriers larger than k_BT is difficult to simulate using the Monte Carlo method. The scattering matrix approach, however, can be applied in the presence of a large potential barrier by dividing the barrier into smaller barriers within each semiconductor slab.

Figure 4 shows the band diagram of the model M-S diode. 20 scattering matrices, i.e. 20 position bins, were used. We were able to simulate electron

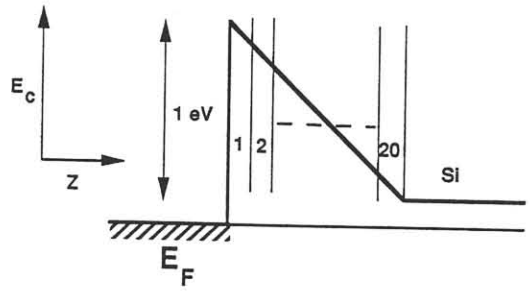

Fig. 4 Band diagram of an M-S diode. 20 scattering matrices are used.

transport against a barrier height of 1 eV using the scattering matrix approach. Conventional Monte Carlo techniques have difficulty with barrier more than a few k_BT high. Statistical enhancements can be used to treat barriers on the order of 0.5 eV high, but the Monte Carlo technique is not well suited for treating very high barriers.

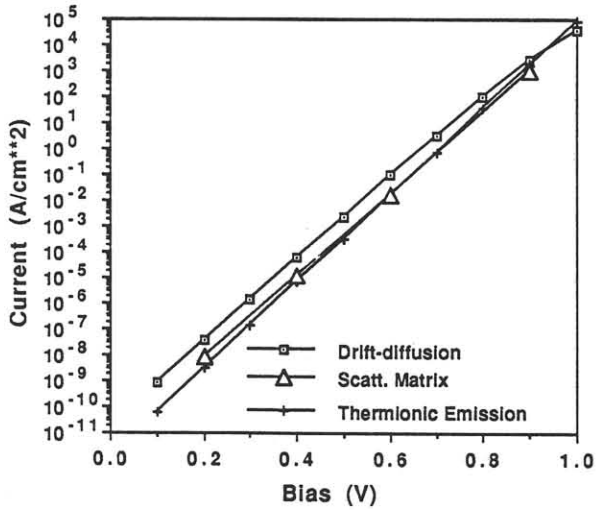

Fig. 5 Current-voltage characteristics of an M-S diode.

Figure 5 shows the I-V characteristics of the M-S diode. At smaller forward bias when the barrier height is large, the net current through the diode is slightly higher than the thermionic emission current, but much smaller than the diffusion current. Some electrons, which otherwise would be reflected by the barrier, absorb a phonon and gains sufficient energy to go over the barrier. These electrons make the total current slightly

higher than the thermionic emission current [5]. At higher forward bias, the total current is higher than the thermionic emission current and it follows very closely the thermionic emission diffusion theory (TED) predictions. This simulation shows that although the validity of the TED theory under high field in the depletion region is questionable, it can predict the total current very well. The effect of absorption of phonon is found to be insignificant when the total current is large at higher forward bias.

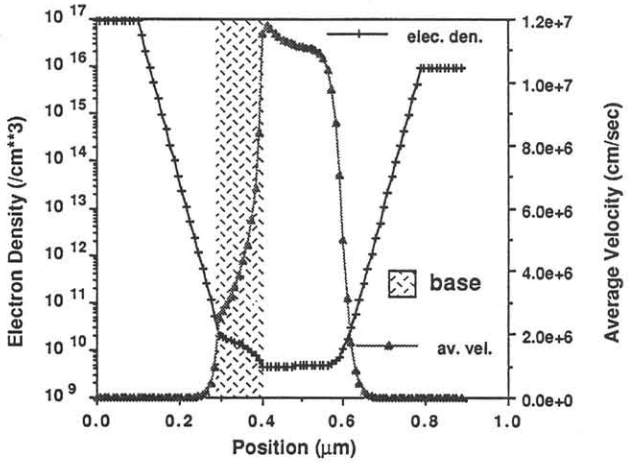

Fig. 6 The figure shows the average velocity and electron density versus position across a model transistor structure.

We also simulated a model p-n diode by the scattering matrix approach. The quasi-neutral region in the diode is represented by a set of zero-field scattering matrices, and the SCR region is represented by the set of scattering matrices computed for the barrier in the M-S diode. We found the scattering matrix results agree with the drift-diffusion calculations.

Finally, we have combined the knowledge gathered from simulating accelerating-, zero-, and decelerating-field regions, and have simulated the simple, model transistor structure shown in Fig. 6. For this structure, we assumed a uniform electric field in the emitter-base and base-collector SCR's. The variation of the average velocity along the transistor structure shows the diffusion effects in the base where the average velocity increases to maintain current continuity since electron density decreases as the distribution of carriers diffuses through the quasi-neutral base. Velocity overshoot effect is present right at the onset of the base-collector space charge region. A study of the average energy of carriers shows that the electrons remain in thermal equilibrium until the distribution of carriers sees the high electric field in the base-collector SCR. We should stress that this is a simple model transistor to illustrate the approach, but it demonstrates that the scattering matrix approach is suitable for treating advanced bipolar transistors.

4. Conclusion

We have demonstrated that the scattering matrix approach is capable of simulating advanced devices beyond the drift-diffusion framework. The next step is to extend the scattering matrix approach to more realistic structures.

Some of the key advantages of the scattering matrix approach are: a) the physics of carrier transport is considered when computing scattering matrices. A device simulation engineer can use pre-computed scattering matrices without worrying about the complex physics involved in computing them, b) hybrid simulation is possible by computing scattering matrices using different techniques. c) recombination of carriers can be treated [3]. At present, we treat only steady state, and carrier-carrier scattering is neglected. These two limitations, however, can be removed at the expense of higher CPU time.

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References

[1] W. Lee, S. laux, M. Fischetti, and D. Tang, *IEDM abstract,* 473, 1989

[2] A. Das and M. S. Lundstrom, To appear *in Solid-State Electronics.*

[3] J.P. McKelvey, R.L. Longini, and T.P. Brody, *Phys. Rev.,* **123,** 51 (1961).

[4] C. Jacoboni and L. Reggiani, *Reviews of Modern Phys.,* **55,** 645 (1983).

[5] T. Wang, K. Hess, and G. J. Iafrate, *J. Appl. Phys.,* **58,** 857 (1985).