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Theoretical Tools for Semiconductor Devices

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Abstract

This is the final report of a three-year, Laboratory-Directed Research and Development (LDRD) project at the Los Alamos National Laboratory (LANL). Future generations of Very Large Scale Integrated (VLSI) circuits require semiconducting devices that are much faster and smaller than current devices. Three-dimensional and transient effects are critical to the performance of these devices. Yet using Monte Carlo (MC) codes to perform time-dependent, three-dimensional simulations will not be feasible in the foreseeable future. Here we re-analyze the physics of semiconductors; use singular perturbation techniques to derive the reduced-dimensionality equations that accurately describe the semiconductor in the regimes corresponding to ultra-small ultra-fast devices; and validate the resulting theoretical models against MC simulations and experimental data. The objective of this project was to gain the capability of accurately simulating ultra-small ultra-fast devices in three spatial dimensions with the ultimate goal of transforming the design of advanced devices.

1. Background and Research Objectives

The scaling of semiconductor devices to submicron lengths is a subject that has recently attracted great interest. Future generations of Very Large Scale Integrated (VLSI) circuits will require semiconductor devices that are an order of magnitude faster and smaller than current devices. Designing these ultra-small and ultra-fast devices will require accurately simulating three-dimensional and transient effects in semiconductors, which are critical to successfully predicting the performance of the new devices [1-7].

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Several crucial issues that are likely to cause severe performance degradation must be considered when scaling semiconductor devices down to the deep submicron regime [4]. In particular, as the feature size of electronic devices continues to shrink, the high electric fields and impurity concentrations substantially modify carrier transport. At fields larger than 10^3 V/cm, silicon and germanium devices become non-ohmic [1-3]. At such fields the charge carriers in a semiconductor are accelerated far above their thermal-equilibrium energy (given by the lattice temperature). Under this circumstance so-called "hot electron effects" become important and many of the familiar concepts of semiconductor physics lose their validity. For very small lengths and high fields, previous drift-diffusion models, hydrodynamics and energy models, and Monte Carlo simulations with oversimplified energy band structures do not provide a satisfactory description of carrier transport and hot electron degradation. Until now, no reliable models relating carrier heating in the semiconductor to actual degradation processes have been developed for ultra-small devices under high electric fields.

Much effort has been dedicated to answer the question of what is the correct description for carrier transport in high electric fields. The dynamics of carriers (both electrons and holes) in semiconductors can be described in terms of wave packets that have semiclassical equations of motion. These equations can be written as:

$$dx/dt = v = \text{grad}_k E_n(k)$$

$$dk/dt = F(x)$$

where v is the group velocity of the wave packet with wave number k , x is the mean position of the wave packet, and $F = eE/h$ is the driving force. Here, E_n is the n -th eigenvalue of the Schrodinger equation associated with the n -th wave packet of wave number k , and it represents the energy of the carrier in the band n . Both x and hk are sought as describing the carrier position and momentum respectively, which are the dynamical variables of effective "semiclassical" particles. The wave number k is restricted to the first Brillouin zone. The conceptual picture associated with those wave packets is that of a "gas" of carriers driven by the electric field and carrier-carrier interactions, and scattered by thermal vibrations of the lattice (phonons) and impurities of the semiconductor. The dynamics of the semiclassical carriers can be described using a Boltzmann transport equation (BTE) or simulated using Monte Carlo (MC) techniques.

The semiclassical description given by the BTE is believed to provide an appropriate description of the physical mechanisms present in most current semiconductor devices. In principle, electronic properties of semiconductors can be predicted very accurately from the BTE that expresses how the carrier distribution evolves in the phase-space of the semiclassical dynamical

variables (position and momentum) describing the carriers. Obtaining direct numerical solutions of the BTE has proven to be exceedingly slow due to its high dimensionality (time, three space coordinates, and three momentum coordinates).

On the other hand, accurate MC simulations require enormous computing resources that are usually incompatible with the requirements for day-to-day device design in industry [1, 2, 6]. State-of-the-art MC programs are usually limited to steady-state simulations in two space dimensions. Even then, a supercomputer may take many hours to simulate a single device. It should also be stressed that the results of MC simulations can vary widely even when they are applied to the same example problem [1]. Recently, it was shown [1] that most MC codes produce results that are strongly correlated with the particular approximations and numerical algorithms involved. Even the latest efforts using MC techniques to model the physical processes driving the carriers [e.g., DAMOCLES (IBM) and SLAPSHOT (University of Texas)] produced phonon-limited mobilities that differ from the experimental values. None of the MC approaches have yet matured to a degree where they can be used in an engineering environment. This indicates that, in spite of the large computing power used, the physical models of carrier transport have to be improved beyond the accepted "state of the art" in device simulation.

Our goals were to develop improved two- and three-dimensional ensemble MC simulation capabilities and accurate, engineering oriented, models to simulate carrier transport. More precisely, our goals were to:

- Develop an accurate model for carrier transport in semiconductor devices based on existing models. Evaluate its applicability and efficiency to predict transport in submicron devices. Study the basic physical mechanisms involved in driving the carriers and their effects on transport.
- Implement the model by developing efficient reduced-dimensionality codes, MC codes and algorithms in one, two and three dimensions.
- Develop an engineering-oriented model, compatible with the day-to-day simulation requirements of the microelectronics industry, based on our previous models. This model will provide the essential features of submicron device transport.
- Test the engineering oriented model with various MC results and hydro-models available in the literature.

Our current MC code includes the largest amount of "first-principle physics" compatible with reasonable computational resources. We included a detailed energy band structure for the carriers, more realistic phonon dispersion relations than the ones found in most MC codes, and introduced appropriate models for impurity scattering and impact ionization mechanisms. The code is based on MC simulation of semi-classical carriers driven by self-consistent electric fields, carrier-acoustic and optical phonon scattering, carrier-carrier scattering, carrier-impurity scattering, and

mechanisms for carrier creation (impact ionization). Accurate tables for calculating the scattering rates, the overlap integrals and the energy band structure of diamond-type crystals are determined from pseudo-potential calculations, resulting in a detailed description of the carrier transport properties.

Our MC code and reduced dimensionality models provide a flexible and powerful means for carrying out transport simulations for semiconductor device modeling. It represents an important simulation capability that can be used as a reference against which other, engineering-oriented, reduced-dimensionality models can be tested.

2. Importance to LANL's Science and Technology Base and National R&D Needs

Los Alamos is engaged in critical research projects to develop the theoretical and numerical tools needed to design and manufacture advanced devices for the next generation of VLSI microelectronics. This capability is vital to maintain the country's competitive edge in the microelectronics industry, which is essential to both civilian industries and defense programs.

Critical elements of this project were deriving accurate mathematical models of transport and writing computer codes to validate these models. Successful completion of the project required extensive simulations of carrier transport in semiconductor devices and a deep understanding of kinetic transport theory and boundary layers.

With the results obtained, we expect to gain the capability of accurately predicting the steady-state operation of advanced devices in three spatial dimensions, and simulating their time-dependent behavior in two dimensions. Such capabilities will greatly enhance US industry's capability for designing advanced VLSI computer chips effectively, enabling industry to bring out next-generation chips more quickly and efficiently.

3. Scientific Approach and Results

Our approach was to develop an ensemble MC code which includes the largest amount of "first-principle physics" compatible with the computational resources available. The code is based on MC simulation of semi-classical carriers driven by self-consistent electric fields, carrier-acoustic and optical phonon scattering, carrier-carrier scattering, carrier-impurity scattering, and mechanisms for carrier creation (impact ionization) and boundary effects like carrier scattering due to surface roughness. Accurate tables for calculating the scattering rates, the overlap integrals and the energy band structure of diamond-type crystals are determined from pseudo-potential calculations, resulting in a detailed description of the carrier transport properties. However, the method to determine the

final momentum after a collision has yet to be optimized by introducing some improved algorithm. In addition, we explored the possibility of introducing some carrier nonlocality effects and localized impurity effects, which are missing in most MC codes and reduced-dimensional models. These effects have been addressed as key issues for extremely small devices. Additional work should be done in this area to elucidate the relevance of these effects. Quantum effects occurring in submicron channels or in inversion layers will also have to be incorporated since it is believed that they can affect transport significantly.

Instead of using the Brillouin zone (BZ), we introduced a re-mapped Brillouin zone (RBZ) where two of the reflection-permutation symmetry operations are replaced by a shift of the carrier momentum to the closest point $G = (0,0,0)$ or any equivalent point to $G' = (1,1,1)$. The RBZ algorithm reduces the number of calculations needed to re-inject carriers leaving the Brillouin zone since the re-mapped Brillouin zone is a quasi-periodic rectangular prism (see figure). To save memory, we also used the symmetries of the BZ, storing the band structure and scattering rates only in the irreducible 1/48th wedge. The irreducible wedge is divided into three tetrahedra described with nonuniform grids. The reduction of the carrier momentum to the irreducible wedge using symmetry operations takes little CPU time since it is performed by a series of axis permutations and reflections, and no three-dimensional matrix manipulation is needed.

During the course of this LDRD project we:

- Developed a realistic model to predict the transport of carriers in submicron semiconductor devices for high fields.
- Derived a model suitable to simulate three-dimensional steady-state and two-dimensional time-dependent semiconductor devices for moderate and high electric fields.
- Developed accurate reduced-dimensionality models based on our previous models [7].
- Assessed the potential of MC codes to test reduced-dimensionality models.

The reduced-dimensionality models and Monte Carlo code we developed provide a flexible and powerful means for carrying out transport simulations for semiconductor device modeling. They represent an important simulation capability that can be used as a reference against which other, engineering-oriented, reduced-dimensionality models can be tested.

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Electron distribution in momentum space at (a) 10 kV/cm, (b) 100 kV/cm, and (c) 1 MV/cm electric field along the $\langle 100 \rangle$ direction at 300 K. At 10 kV/cm, most of the electrons reside in the sixfold equivalent X valleys. At 100 kV/cm, they are still confined in the X valleys, but widely distributed. Note that the centroid of electrons in each valley shifts slightly against the electric field, which gives rise to a finite drift velocity. At extremely high fields like 1 MV/cm, the electrons are distributed in the entire Brillouin zone, indicating a high average energy.

Figure 1

Re-mapped
Brillouin
Zone

Figure 2