MONTE CARLO SIMULATION OF SILICON DEVICES

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Introduction

The Monte Carlo method is a well established approach for the statistical solution of the Boltzmann transport equation in semiconductors [1, 2]. As device dimensions are reduced, it is important to account for hot electron effects, responsible for overshoot phenomena and reliability problems like breakdown due to impact ionization, defect generation, and injection into gate oxides. In some cases, hot electron effects can be used in a controlled fashion to generate useful device functions, as is the case of floating gate memories. Reliable models for the simulation of advanced MOS structures must include the complete details of the bandstructure and accurate models for scattering rates at high energies, as well as a self-consistent treatment in order to evaluate appropriately the space-dependent carrier distribution function.

Applications of full-bandstructure Monte Carlo approaches to realistic geometric structures have become feasibile only very recently, thanks to the advances in supercomputers and high end workstations. An example is the simulator DAMOCLES [3, 4] developed at IBM, Yorktown Heights. The ongoing goal of our work is to develop a hierarchy of models, where the features of the band structure in the high energy range can be introduced with increasing complexity, so that full device investigation may be practical. The most complete model in the hierarchy includes a full k-dependent description of the scattering rates. The computational requirements are enormous and todate such an approach is practical for the investigation of bulk phenomena. Applications on massively parallel computers could be a solution to make this approach more viable in the future for full device simulations. A step below in the hierarchy is a model where scattering rates only depend on energy. The main difference of this model with respect to traditional Monte Carlo approaches, with an analytical bandstructure formulation, is in the use of the full bandstructure to calculate numerically the particle trajectories in momentum space and to determine the final state after scattering.

This talk will introduce the issues related to practical Monte Carlo simulation of silicon devices, using a full bandstructure approach, and will discuss the implementation and representative results of a self-consistent simulator based on energy dependent scattering rates.

The Monte Carlo Model

The knowledge of the band structure is necessary in order to solve the equations of motion

$$\frac{d\mathbf{r}}{dt} = \frac{1}{\hbar}\nabla_{\mathbf{k}}E(\mathbf{k}) \tag{1}$$

$$\frac{d\mathbf{k}}{dt} = \frac{e\mathbf{F}(\mathbf{r})}{\hbar} \tag{2}$$

where $\mathbf{r}$ is the electron's position, $\mathbf{k}$ is the electron's wave vector, $E(\mathbf{k})$ is the energy, $\mathbf{F}(\mathbf{r})$ is the local electric field, and e is the elementary charge. The band structure gives detailed information

on the energy and velocity of the electron as well as the correct density of states.

In typical Monte Carlo simulators, the non-parabolic approximation is used to describe Si

$$\frac{\hbar^2}{2m_o}\left(\frac{k_x^2}{m_x}+\frac{k_y^2}{m_y}+\frac{k_z^2}{m_z}\right)=E(1+\alpha E) \tag{3}$$

where m_o is the free electron mass, m_i is the effective mass in the i^{th} direction, E is the energy, and α is the non-parabolicity factor. Using the Herring-Vogt transformation [5], the ellipsoidal isoenergy surfaces are transformed into spherical ones. This approximation is only valid near the bottom of the valley for a single band.

For high energy transport, the non-parabolic approximation does not adequately describe Si. First, the second conduction band is degenerate with the first conduction band at the X point with an energy of approximately 130 meV. Second, at higher energies, the band structure of Si just cannot be described by such a simple expression (for example, at the Γ point).

In our simulator, the band structure for Si is calculated using the empirical pseudopotential model of Cohen and Bergstresser [6]. The energy and gradient (for the calculation of velocity) is calculated for the k points inside the irreducible wedge of the Brillouin zone (BZ), described by

$$0 \le k_z \le k_x \le k_y \le 1 \tag{4}$$

$$k_x + k_y + k_z \le \frac{3}{2} \tag{5}$$

Using the symmetry properties, each point in the BZ can be mapped into the irreducible wedge.

Our Si model includes the following phonon scattering mechanisms: intravalley acoustic phonon scattering, F and G type X-X intervalley phonon scattering, X-L intervalley phonon scattering, ionized impurity scattering, and impact ionization. Ridley's statistical screening is included in the ionized impurity scattering [7]. Finally, the total scattering rate is adjusted so that at high energies, it follows the total density of states [8].

Simulations

The initial electron distribution in real space is taken to be proportional to the doping concentration of each region. Thermal equilibrium is assumed for the initial k-state distribution. The random time of flight for the electrons is generated using the modifled constant time technique (MCTT) [9].

At the beginning of every iteration, the electron density in real space is evaluated using a 2D cloud-in-cell scheme [10], and Poisson's equation is solved numerically using the Red-Black Successive Over Relaxation (SOR) method [11]. Holes are included in the constant quasi-Fermi level approximation [3]. Dirichlet boundary conditions are imposed at the source, drain, gate, and substrate contacts, and von Neumann boundary conditions are imposed at the "floating" boundary regions of the device. Also, the boundary layer in the contacts are kept neutral by injecting the necessary number of electrons. The electrons are then allowed to fly ballistically, scatter, or cross region boundaries during a preset time interval δt. This procedure is repeated until a specified convergence criterion is met.

In Fig. 1 we show for demonstration some representative results of Monte Carlo simulations for a simple $n-$channel MOSFET structure, obtained with the full band model using energy dependent scattering rates. We assume a uniform acceptor doping $N_A = 10^{16}\ cm^{-3}$ in the $p-$substrate and

contact regions with $N_D = 10^{19}\ cm^{-3}$. The number of simulated particles fluctuates in excess of 15,000 according to the bias. Figure 1(a) shows a portion of the I-V characteristics for a 1 μm gate device, which were obtained to check code calibration. These results are very close to drift-diffusion solutions from . the PISCES IIB simulator. Fig. 1(b) shows the deviation of the drain current from a linear scaling rule when the gate length is reduced. The potential profile in the conduction channel of a 0.25 μm gate device, in Fig. 1(c), shows that flat potentials are established in the contact regions. With a lower doping concentration in the contacts to reduce the number of simulated particles and computational cost, the simulation would yield fairly large fields in the contact regions. Figure 1(d) shows the energy particle distribution, obtained at the channel-drain junction with the same structure and bias of Fig. 1(c). The reference zero energy for all particles is the bottom of the $X-$valley. The ability to generate the electron distribution function is the main feature which distinguishes the Monte Carlo procedure over other established simulation techniques. All the examples shown were run on Hewlett-Packard 700-series workstations, requiring several hours per bias point, demonstrating that a full bandstructure Monte Carlo approach should be considered practical and affordable.

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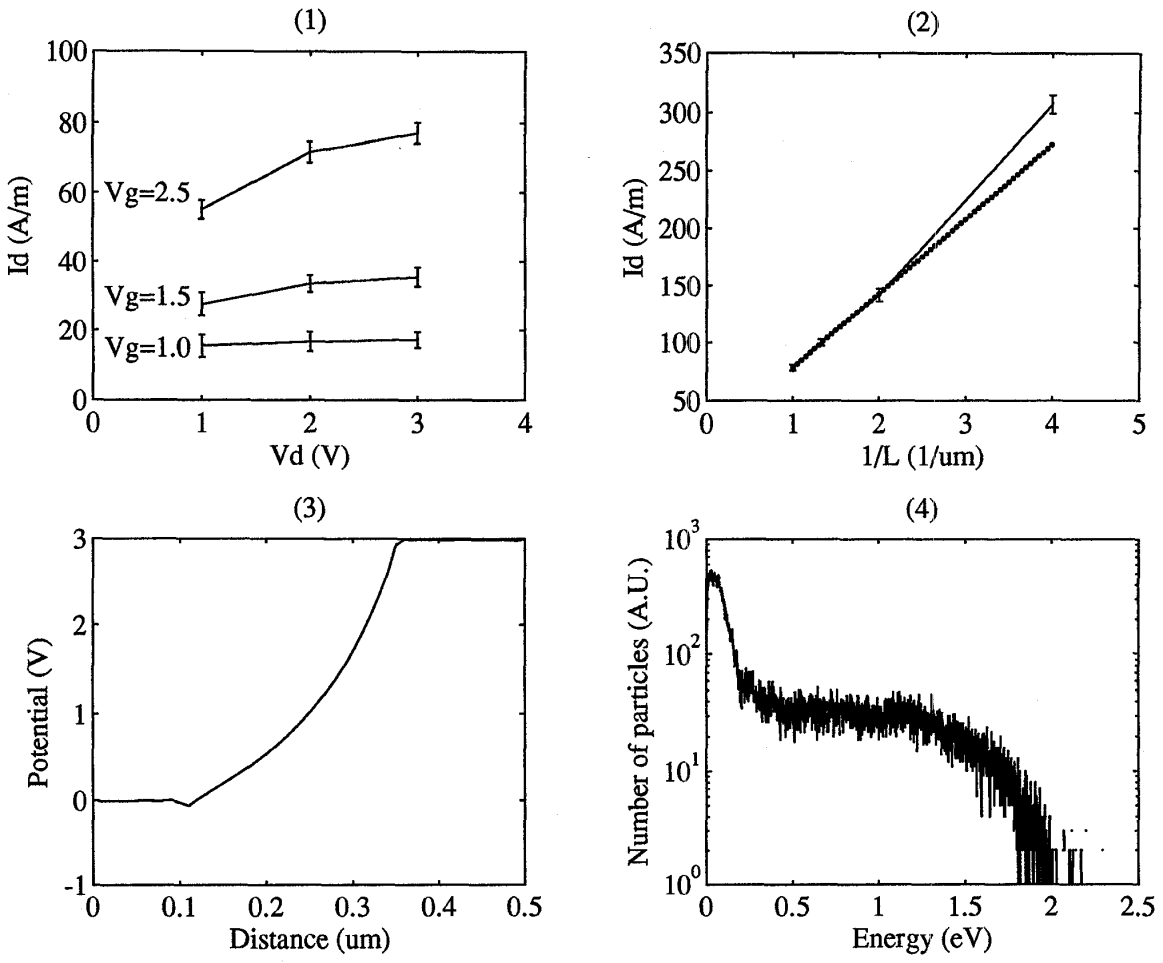

Figure 1.

(a) I-V characteristics of a conventional 1 μm MOSFET.

(b) Drain Current vs. the reciprocal of the channel length 1/L, with Vgs=2.5 V and Vds=3.0 V. The dotted line is the linear extrapolation of the drain current.

(c) Electrostatic potential profile of a 0.25 μm MOSFET in the channel. Vgs=2.5 V, Vds=3.0 V and t_{ox}=600Å

(d) Distribution of particles at the channel-drain junction for a 0.25 μm MOSFET. Vgs=2.5 V, Vds=3.0 V and t_{ox}=600Å.

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