

## MONTE CARLO SIMULATION OF SEMICONDUCTOR DEVICES AND PROCESSES

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### SUMMARY

A critical discussion of the Monte Carlo simulation as applied to semiconductor device and process modelling is presented. The advantages and limitations of such approach are discussed and compared with more traditional simulators. Critical points are pointed out and analyzed. A variety of applications is then outlined.

### INTRODUCTION

The Monte Carlo method (MC) can be considered as a very general mathematical tool for the solution of a great variety of problems [1-4]. In its present form, the method is attributed to Fermi, Von Neumann, and Ulam, who developed it for the solution of problems related to neutron transport.

Among the various applications of the method the following are probably the most important:

- \* Integro-differential equations
- \* Matrix inversion
- \* Transport of nuclear particles
- \* Transport in semiconductors
- \* Modeling of semiconductor devices
- \* Process simulation

Being based on random numbers, the results obtained with a MC procedure are never exact, but rigorous in a statistical sense: the exact result lies in given intervals with given probabilities. The applications of MC methods can be divided into two major groups. One consists of direct reproduction on a computer of the microscopic dynamics of the physical

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process in a system which is already statistical in its nature. We use in this case the term "MC simulation". The second group consists of MC methods devised for the solution of well defined mathematical equations. In such cases the methods are used to solve the equations that describe the problem of interest.

The two applications of the MC that we will focus on are particularly important in light of the terrific growth in the field of microelectronics achieved in recent years. Semiconductor devices are nowadays built with their active dimension below one micron. The reduction in size leads to a higher integration level as more devices can be put into a single chip. Moving into the submicron scale, many new physical phenomena become important that require a sophisticated theoretical treatment. Furthermore, new possibilities for revolutionary devices are offered by the capability to grow nanometer layered structures with extremely high quality by molecular beam epitaxy (MBE) and Metal organic chemical vapour phase epitaxy (MOCVD). There is therefore a new challenge towards the understanding of the principles of operation of those novel devices. As we will see, the MC method offers great advantages in this direction.

On the other side, the push towards smaller and more powerful devices (which immediately translate into higher levels of integration and enhanced performance of the single devices as well as of the overall circuit) has been sustained by enormous advances in the area of fabrication and processing. A very precise control is nowadays possible on the device geometry and doping profile through techniques such as ion implantation, reactive ion etching, electron and X-ray lithography.

Computer programs are extremely important for technology development. Computer Aided Design (CAD) has become one of the keywords in microelectronics. The importance of such field can be greatly appreciated focussing on the steps required for the fabrication of integrated circuits (IC) [5]. There, the development of new technologies has been driven by an experimental approach. A useful alternative was offered by software tools, which can lead to a speed up of the development cycle and a reduction of the development costs. In fact, those calculations can be considered as simulated experiments, which can be much faster and less expensive than real experiments. Furthermore computer experiments allow a deep physical interpretation of the final results that leads to a better understanding of the problem at hand. This is particularly true for the MC simulations.

The characteristic links between the different aspects of CAD can be summarized as follows [5]. The output of the process simulation is fed directly into a device simulation program, which determines the electrical characteristics and the performance of the device. At this stage, the interplay between process and device simulation can suggest improvements on the processing steps deduced from the simulated device performance. The output of the device simulator is then compacted to be inserted in a circuit simulation program, which determines the characteristics of the overall circuit. As we will see in the following sections, MC simulators are finding wider and wider use as CAD tools.

Although it will not be possible to exhaust the complexity of the MC

simulation of devices and processes in such a short review, the present paper is intended to give a critical overview of the MC algorithm for device and process modelling. The next session will deal with the MC simulation of semiconductor devices. A short description of a generic MC simulator will be given, together with special features that are needed for the simulation of very complicated systems. A complete overview of the Monte Carlo simulation of semiconductor devices will be presented in a forthcoming book [6]. The third section will focus on MC process simulations. Some specific examples will be presented. The areas of processing where the MC simulators are preferable to other approaches will be discussed.

## SEMICONDUCTOR DEVICE SIMULATION

The Monte Carlo technique is a fairly new tool in the area of device modeling, traditionally dominated by simulators based on drift-diffusion or on balance-equation models (for an overview of the subject see Ref. 7,8). The application of MC techniques to the simulation of semiconductor devices started quite soon after the introduction of the method [9,10] but has received great attention only recently [11,12] since it requires very large amount of computations, made possible only by the most recent computers. With the recent advances in material growth, contact deposition and impurity control, devices have become more transparent from the physical point of view. Incidentally, this has provided physical systems of extreme interest. At the same time, MC algorithms have gained in sophistication and are now able to handle phenomena and systems of great complexity. These are two fundamental steps since the necessary input for a MC simulation of semiconductor materials and devices is the physical system under investigation. Many semiconductor devices can be nowadays simulated with the MC method, which is becoming more and more a very useful modeling tool.

The most common (and also the most interesting) simulation of a semiconductor device is performed for many particles in parallel (Ensemble Monte Carlo) and coupled to Poisson's equation in order to obtain the self-consistent potential consistent with the charge distribution given directly by the Monte Carlo procedure. For system of great complexity, a one particle Monte Carlo (OPMC) simulation can be performed on a given fixed potential previously determined.

Since no a-priori assumptions are needed on the form of the real and  $\mathbf{k}$ -space carrier distributions, a Monte Carlo simulator is the only reliable tool for the investigation of those physical phenomena that critically depend on the shape of the distribution, or on the details of its tail (such as electron injection over potential barriers). Furthermore, the Monte Carlo technique allows us to focus on particular physical mechanisms that might be of importance on the device performance (for example, intercarrier scattering, impact ionization, generation-recombination, etc.). The prices one has to pay are a very time-consuming algorithm, and the requirement of a complete knowledge of the physical system under investigation. Often many assumptions have to be made in order to reduce the complexity of

the model describing a given device.

### The Monte Carlo algorithm

In recent years the Ensemble Monte Carlo (EMC) has been widely used to study the properties of semiconductor devices. Particular emphasis has been lately attributed to submicron structures, because of their performances in switching and high frequency operations [13]. Once the basic physics involved in the transport of such devices is known, EMC simulation provides a formidable tool to determine their limits and characteristics and can be very helpful in modeling. Together with the determination of the macroscopic properties of a device, EMC also gives a microscopic description of the local electric field, charge density, velocity distribution, etc. An excellent overview can be found in Ref. 14.

A flow chart of a generic EMC self consistent device simulation is shown in Fig. 1. The basic steps are :

i) Set up geometry and discretization scheme; two parameters that play an important role in the choice of the time step and the grid size are the plasma frequency and the debye length [14].

ii) Charge assignement. The charge of each particle is assigned to a particular mesh point. Since it is not possible to simulate all the electrons present in a real device, each simulated particle represents a cloud of electrons for the purpose of estimating currents, charge and field distributions. For all other purposes, each individual particle carries its elementary charge  $e$ . The doping charge is also added to the mesh according to its distribution. Although the EMC simulation is inherently three dimensional, we usually deal with one or two dimensional grids. In such contest the assumption is the perfect homogeneity in the dimensions that are not considered explicitly.

iii) Potential solution. Poisson's equation is solved to determine the electrostatic potential at the mesh points. In connection to EMC simulations, a finite difference scheme is generally used. The solution can be obtained in several way, the most efficient being the Fourier Analysis Ciclic Reduction (FACR) and the direct matrix inversion. The former method provides a very effective algorithm that allows the inclusion of special boundaries through the so called capacity method. The latter requires a matrix inversion at the beginning of the simulation. The new potential is calculated with a simple matrix multiplication at fixed times during the simulation. Such method is particularly efficient on computers with vector processing. The electrostatic field is then obtained from the potential with a finite-difference algorithm.

iii) Flights. Each particle, now treated as an individual electron, undergoes the standard MC sequence of scatterings and free flights, subject to the local field previously determined from the solution of Poisson's equation. The MC sequence is stopped at fixed times, when the field is adjusted following the steps described above. For OPMC techniques, the potential and field profiles are calculated at the beginning of the simulation, and only step iii) is performed.

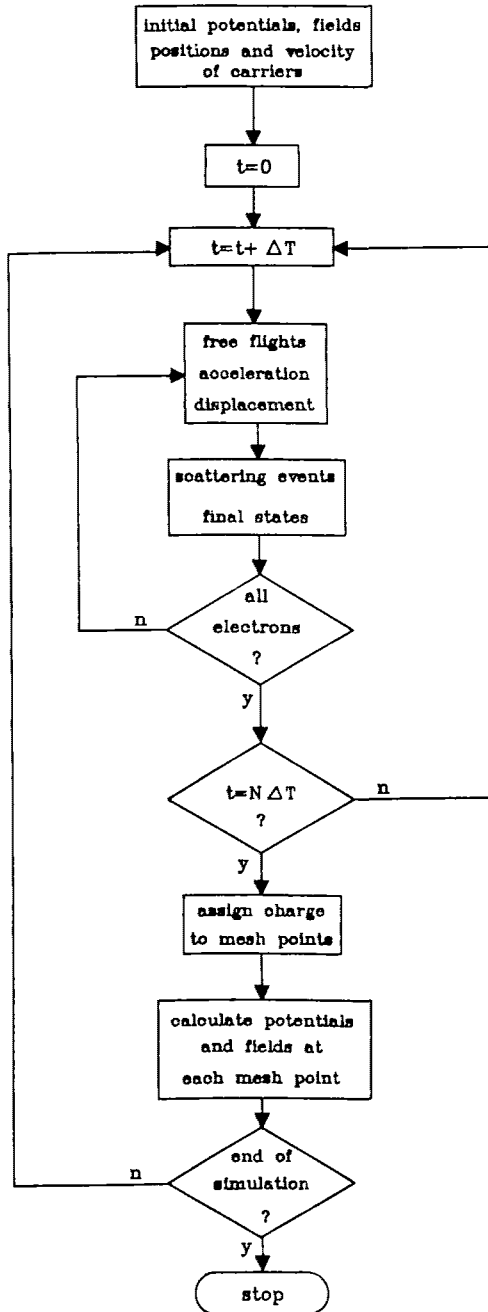


Fig. 1 Flow chart of a typical MC program for device simulation

The description of the problem is completed by setting initial and boundary conditions. The initial conditions are not so important, since only the self-consistent steady-state result is usually retained. Boundary conditions are instead crucial, in particular in submicron devices, where contact properties drastically influence the whole behavior of the device. We will return to this point later.

Traditionally, device simulators have been based on drift diffusion (DD) or on balance equation (BE) models. Both of them are fast and reliable as long as a local description of the physical phenomena in the device is possible. That is, when the carriers can be described by a distribution characteristic of the given field present in every of the device. Such an assumption breaks down when the device dimension are small (typically below one micron), and high fields set up, leading to non-local phenomena. More specifically, when the field inside the device varies appreciably over length comparable with the electron mean free path, the electrons at a given position carry information about the field value at another position, and the transport process becomes a non local phenomenon. The inclusion of the energy balance equation allows to incorporate some of these effects, at the cost of a much heavier computation [8,12]. The Monte Carlo technique, which is inherently non local, lends itself very well to the simulation of non stationary transport in devices. The discrepancy between local models and the EMC have been clearly outlined by several authors [15-17].

Examples of MC simulators present in the literature can be found in refs 18-29. The prototype, and hystorically the first self consistent MC program, was applied to a MESFET structure by Hockney and coworkers at Reading University [14,15]. These algorithms have been so successful that they are adopted by most of the self consistent MC programs. Typical MC results for a  $0.25 \mu m$  GaAs MESFET operating at room temperature are shown in Figs. 2 and 3 [29].

A large class of devices (MOSFET, bipolar transistors, HEMTS, etc) are characterized by areas with high doping (and free electron) concentrations, low electric field and retarding barriers. The direct simulation of electronic motion in these regions can be terribly time consuming. In contrast, more traditional simulators, such as (DD) schemes, can be applied to such a situation in a reliable and straightforward way. A hybrid method (HYMC) has been proposed [30,31] that combines the two techniques, by relying on the fast DD simulators for low field areas, and on the direct MC simulation where steep gradients of the potential create the condition for hot carriers. Although excellent in principle, the hybrid technique (also called regional MC) requires a very accurate handling of the boundary conditions at the interface between the various region which, in our opinion, has not yet been obtained.

### Special Features

In the following section, we focus on special aspects of the MC simulation that are non generally considered because of their difficulty, although

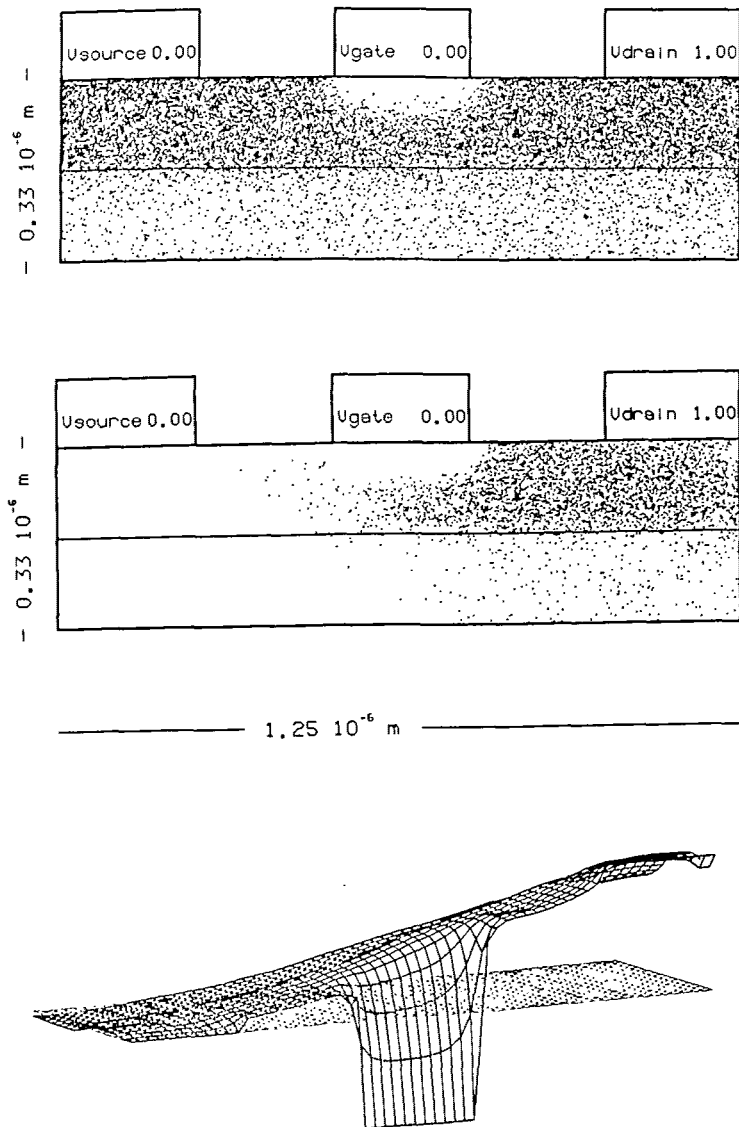


Fig. 2 Electron distribution inside a quarter micron gate MES-FET showing all the electrons (a) and only the  $L$  valley electrons (b). The potential distribution is shown in (c). The operating conditions are zero bias on the gate, and 1 V on the drain. The epilayer is doped at  $10^{17} \text{ cm}^{-3}$ , the substrate at  $5 \times 10^{15} \text{ cm}^{-3}$ . The continuous line indicates the boundary between epilayer and substrate. The simulation has been performed using 20,000 electrons.

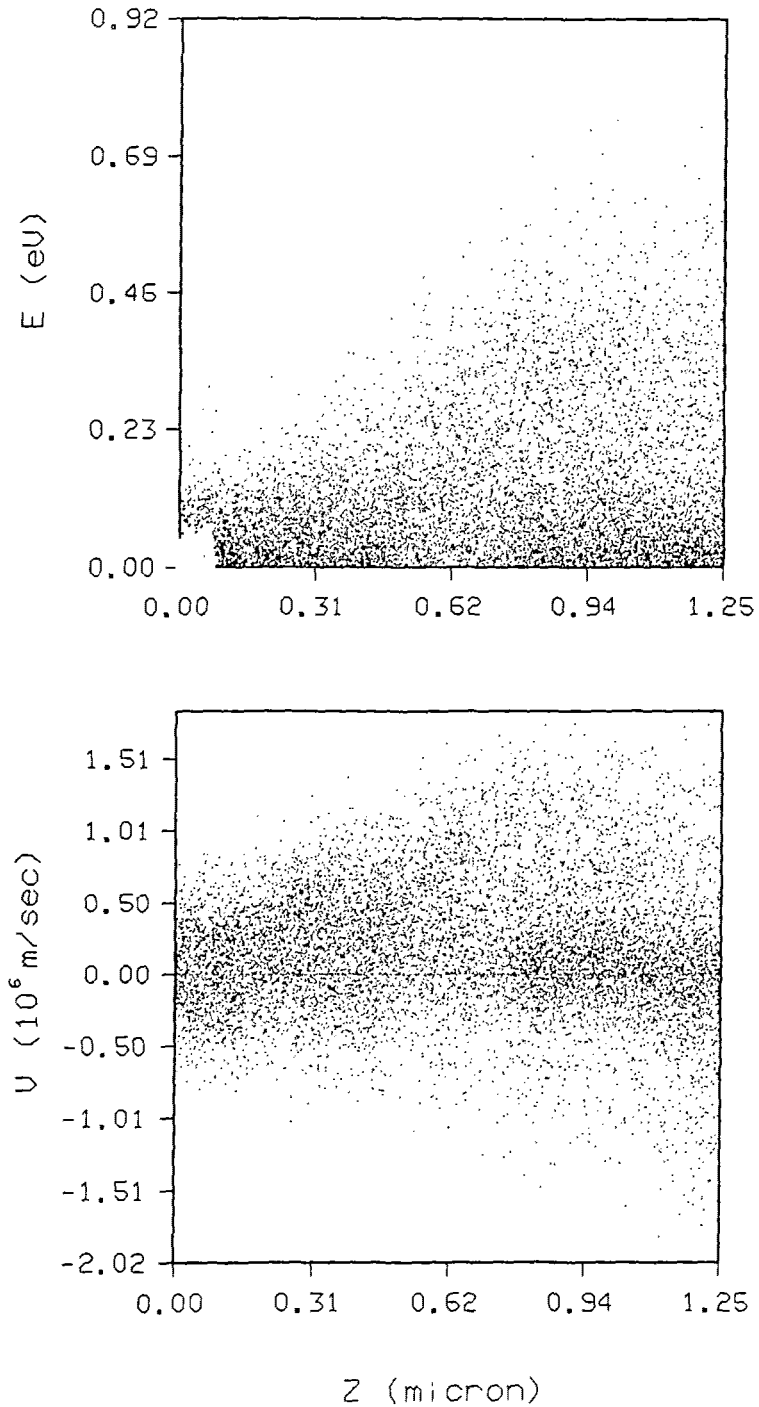


Fig. 3 Total energy (a) and longitudinal velocity (b) distributions for the device shown in Fig. 2.



they can be of great importance in the device performance.

### Pauli Exclusion Principle

Electrons obey the Fermi-Dirac statistics and then must satisfy the Pauli Exclusion Principle. This means that not all the states are available because only one electron can reside in each state. This aspect is not very important in nondegenerate case and electrons are distributed in a large interval of states; in the degenerate case the problem becomes more conspicuous. In GaAs the electrons are degenerate for  $T \leq 300K$  and for  $n > 4.6 \times 10^{21} m^{-3}$ . This is the case for many devices of interest. Degeneracy is equivalent to a many body interaction which reduces the phase space available for the electron final state in an induced transition.

If  $p(\mathbf{k})$  and  $p(\mathbf{k}')$  are the probabilities that respectively the initial and final state are occupied, the total rate of transition  $P(\mathbf{k}, \mathbf{k}')$  between two different states is given by  $P(\mathbf{k}, \mathbf{k}') = p(\mathbf{k}) \times S(\mathbf{k}, \mathbf{k}') \times [1 - p(\mathbf{k}')]$ . Normally a semiclassical Monte Carlo works with the approximation  $p(\mathbf{k}') = 0$  because all the states are considered available as final states. The inclusion of PEP is then essentially the inclusion of this term in the total scattering rate. In Ensemble Monte Carlo this is obtained very easily because the particle distribution is known step by step. The algorithm generating the distribution function is set up by multiplying the scattering probability by the correction factor  $1 - p(\mathbf{k}')$ ;  $p(\mathbf{k}')$  is determined self consistently and a rejection technique is used after selecting the final state without the correcting Pauli factor [32-33].

### Contact Simulation

The simulation of contacts is one of the most serious problems in MC device simulations, due in part to the limited knowledge of the physics of contacts. On the other side, contacts are of great importance in a number of semiconductor devices, whose applications range from high-speed logic to microwaves. As the dimensions of these devices reach the submicron limit, contacts become the limiting factor for the performance in the ballistic or quasi-ballistic mode of operation.

In general, semiconductor devices do not operate under charge neutrality conditions. The net charge inside the device is directly related through Gauss' law to the flux of the electric field on the boundaries, and consequently to the potential inside the device. Therefore, charge neutrality (that is conservation of the number of particles) cannot be enforced in the simulation. Rather, an appropriate handling of the boundaries is required to simulate a number of electrons that varies in time self consistently with the potential distribution. In a device such as the field effect transistor shown in Fig. 2 the most significant boundaries are at the source, drain and gate electrodes. Source and drain contacts are usually treated as ohmic contact by absorbing all the electrons that hit the electrodes and by injecting a number of electrons which maintains a neutral region in the adjacency of the electrodes [14]. The Schottky barrier at the gate is treated as a perfectly absorbing electrode with a potential

equal to the applied potential minus the barrier height. Although commonly assumed, the above conditions have never really been tested. One attempt to deal with the problem of contacts in a simulation of a 1-D metal- $n-n^+$  structure has been presented in Ref. [34]. This is an interesting system in that the device is never charge neutral, except under flat-band condition. This is due to the presence of a depletion or an accumulation region near the interface. In order to allow the number of the electrons simulated to vary during the simulation, a novel scheme was used, based on a cubic Hermite collocation method to solve the 1-D Poisson's equation. The value of the electric field at the end of the heavily doped region ( $x = 0$ ) is obtained without any loss of precision, and allows to obtain directly the value of the current through that interface. By carefully controlling the flux of the electrons in the two directions, it is possible to update constantly the numbers of electrons simulated, in accordance to the field distribution inside the device. In this way, the interface at  $x = 0$  is modelled as a perfectly injecting contact. The metal contact acts as an absorbing boundary: electrons with energy sufficient to overcome the barrier are injected into the metal.

Tunneling was also included. The tunneling probability for an electron with energy  $\varepsilon$  at a distance  $x$  from the interface is given by

$$T(\varepsilon) \cong \exp -2/\hbar \int_x^w dx 2m^* [qV(x) - \varepsilon]^{\frac{1}{2}} \quad (1)$$

where  $m^*$  is the effective mass,  $V$  the potential seen by the electron, and  $\hbar$  is Plank's constant. As a MC electron reaches the barrier, the tunneling probability is calculated from (1) using a parabolic least square interpolation of the potential  $V(x)$  obtained from the solution of Poisson's equation. A random number was then used to decide whether the electron would tunnel or not. It is important to notice that no assumptions on the electron distribution function near the contact or on the shape of the potential barrier are needed. At room temperature and moderate electron densities, current is provided solely by thermoionic processes. Higher densities cause a narrowing of the barrier, thus increasing the tunneling probability. The method indicated a significant tunnel currents for electron concentrations above  $5 \times 10^{18} \text{cm}^{-3}$  suggesting that the proposed method might be suitable also for the simulation of ohmic contacts.

### Carrier-carrier scattering

Many devices are characterized by very high electron concentrations. In such situation one might have to worry about the possible influence of the interaction among the conducting electrons. A good example is provided by the Tunneling Hot Electron Transfer Amplifier (THETA) [35,36]. This belongs to a series of new devices generically called "hot electron transistors", based on the idea of improving the device performance by injecting fast electrons into thin base regions. In a standard device, such as a MESFET or HEMT, electrons are injected into the channel with a

thermal energy distribution and a small initial velocity. In order to reduce the transit time through the channel or base, it is advantageous to increase their initial velocity. Electrons are then injected into the base with energies some hundreds of meV greater than the thermal energy. The active part of the device consists of a GaAs-AlGaAs-GaAs quantum well, with a very thin (300 Å) and highly doped ( $10^{18} \text{ cm}^{-3}$ ) GaAs base. Electrons are injected into the base by tunneling through the potential barrier between emitter and base, and they are collected as they overcome the barrier between base and collector. There, if the hot electrons could maintain their high speed through the active region of the device, then very good performance (fast switching, high cut-off frequencies) should be expected. On the contrary, it has been suggested, see for example [37], that the interaction of the injected electrons with the base electrons might be a strong source of degradation of device performance. As well as in metals, plasma phenomena can be of great importance also in polar semiconductors [38-39]. Electrons injected into highly doped regions can be scattered by the collective excitations of the electron gas, as well as through normal binary collisions with the other electrons.

Two main contributions to the carrier-carrier scattering can be identified:

- the individual carrier-carrier interaction via a screened Coulomb potential which accounts for two-body short-range interaction;
- the electron-plasmon interaction, which accounts for the collective long-range behaviour of the electron gas. In semiconductors, the plasmon energy at a reasonable electron density can be of the same order of magnitude as the characteristic phonon energies. In a device simulation, the scattering rates for electron-electron and electron-plasmon processes can be tabulated at the beginning of the simulation. Carrier-carrier scatterings are then treated as any other mechanisms in the MC algorithm.

Due to the high doping in the base region, the Thomas-Fermi screening length should be used. To avoid unphysical long range correlations in the electron-electron scattering the partners are chosen, if there are any, in the range of two Thomas-Fermi lengths.

### Optimization procedures

An original, efficient algorithm has been implemented to calculate the appropriate duration of the free flights (depending on the actual carrier status). The method which is based on a space dependent definition of the scattering rate [40], leads to a drastic reduction in the number of self scatterings thus allowing large saving in computation time (more than one order of magnitude compared with the conventional approaches).

The low injection efficiency of electrons from the  $n^+$  source/drain regions into the channel of a MOSFET has been overcome [24,40] by means of the sample multiplication technique suggested in Ref.[41] to deal with rare carrier configurations. A multiplication technique of the same type has been systematically used to reasonably populate the upper tails of the electron distribution with an affordable number of total simulated

particles.

## MONTE CARLO PROCESS SIMULATION

In this section we will look at MC process simulation mainly from the point of view of IC fabrication, since this is certainly the area where simulation plays a fundamental role. Many different interrelated steps contribute to the realization of the final product. Following Penumalli [5], the IC processing steps can be classified into three major categories:

- a) Thermal processing and doping (ion implantation, predeposition, annealing, oxidation, epitaxial growth);
- b) Pattern definition (reactive ion etching, deposition, evaporation, sputtering)
- c) Pattern transfer (optical, X-ray, electron beam lithography)

Setting up mathematical models for each step requires the knowledge of very complex physical and chemical phenomena connected for example with the redistribution of atoms or impurities into a substrate, or the energy exchange between fast projectiles and the substrate they interact with. As we will see in the specific examples, some drastic approximations are made in order to define a tractable model.

As for the case of device simulation, several analytical and numerical approaches exist in the literature that cover all the processing step outlined above [5,42]. The MC technique has been very successful in some applications, especially those where the simulation can be reduced to a series of uncorrelated events describing the trajectory of a projectile against target atoms. This is the case for example of ion implantation, and electron or ion beam lithography. Those applications will be briefly examined later.

A general consideration that can be made is that, once the mathematical model has been simplified, the MC algorithm for process simulation present fewer difficulties than for device simulation. This is due to (i) the fact that no self consistency is required between internal potential and charge distributions, and (ii) the transition probabilities are assumed to be constant between two successive stochastic events. This point will be clearer in the examples discussed below. There, we will concentrate only on ion implantation and electron beam lithography, which represent the most successful application of the MC method to process simulation.

### Ion Implantation

Ion implantation is one of the most important doping techniques for device fabrication, especially for very large scale integration (VLSI) circuits. The successful application of this technique depends strongly on the ability to control the impurity profiles for a variety of implant conditions. In the past, the basic theory to describe the penetration of charge particles into solids was the one due to Lindhard, Scharff and Schiott (LSS) [43]. The LSS theory has been very successful in the prediction of primary ion range and damage distributions in amorphous semiinfinite substrates. Because of its assumptions, it is not applicable to multilayer structures as

often encountered in VLSI processing.

The MC simulation offers the following advantages:

it accounts for implant profile discontinuities at the interface between different layers;

it allows a rigorous treatment of elastic scattering with the different types of atoms in a multiatomic target.

it gives a full implant distribution rather than only a few of its moments; it can include the recoil effect due to atoms that are knocked into deeper layers from the impinging ions.

The MC simulation of ion implantation is performed by following a large number of individual ion histories in a target, each made up of a sequence of collisions with target atoms, and straight free flight between them. Such "binary collision" model might break down at low ion energy, when deflections can occur even at great distances from a target atom. After each free path the energy of the ion is reduced by the amount of the electronic energy loss and by the nuclear energy loss, which is related to the momentum transfer to the target atom occurring during the collision. The history of each ion terminates either when its energy drops below a specified value or when the particle exits the target.

Different physical models can be used for the various phenomena involved in the energy loss processes. An exhaustive review can be found in [44]. A series of optimizations of the MC program have been discussed in [45]. Such optimizations are crucial since (as pointed out earlier) the major limitation of the MC method lies in the amount of computation required to achieve an acceptable statistical accuracy.

Some of the most important features of the MC simulation of ion implantation are its inherent three-dimensionality, the fact that ion backscattering is naturally accounted for, and that both amorphous as well as crystalline targets can be considered. Those distinctive features make the MC simulation the most suitable approach to the study of ion implantation.

### Electron Beam Lithography

Electron beam lithography (EBL) is another very important technique in microelectronics. EBL is the standard way of fabricating masks for optical and X-ray lithography. Furthermore, direct electron beam writing on wafers is the only practical way to obtain ultrasmall linewidths. In EBL, finely focused beams are used to expose polymeric resist layers. The ultimate resolution obtainable is not limited by the characteristics of the incident beam but rather by the electron scatterings with the resist and the underlying substrate. These scatterings, that leads to the so called "proximity effects", can be classified as: a) forward scatterings within the resist; b) backward scatterings from the substrate; and c) backward scatterings within the resist.

The actual process of electron scattering in solids is very complex, and we have to rely on simplified models and numerical techniques to get quantitative results. As for the case of ion implantation, the best

available approach is given by the MC simulation. In fact, the simulation is somewhat similar to the one described previously for the ions. In the simplest model [46], electrons undergo a series of elastic scattering events with the target nuclei. In addition, they suffer energy losses by inelastic scattering processes with the target electrons. The elastic scatterings are modeled using the screened Rutherford cross section. The inelastic losses are accounted for in a continuous way by reducing the electron energy between two successive collision by an amount calculated from Bethe's energy loss rate. Between scatterings, the electrons are assumed to travel in a straight path, whose length is determined by weighting the mean free path by a random number uniformly distributed between 0 and 1. The sequence of free paths and scatterings is repeated until the electron come to rest. Contrary to the ion case, for EBL the quantity of interest is the deposited energy rather than the position where the particle comes to rest.

Several improvements have been suggested to the simple model described above. In particular, it was pointed out [47] that the production of secondary electrons as a result of a ionization process caused by the incident beam should be accounted for. Since the energy deposition is inversely proportional to the electron energy, the contribution of the secondary electrons (which are slower and move in a direction almost perpendicular to the primary electrons) can be significant. The new hybrid model includes therefore a discrete energy loss mechanism correspondent to the ionization in addition to the continuous energy loss already described. Another improvement is necessary when multilayer structures are considered [48, 49]. Then the length of the free paths has to be determined taking into account the details of the electron dynamics, that is the possibility for an electron to cross one or more layers during its path. Finally, a further refinement of the model has led to the use of Mott cross section rather than Rutherford's one for the treatment of elastic scattering [50].

The MC simulation, combined with resist modeling, has become an extremely powerful tool for the investigation of proximity effects, and has been found in excellent agreement with experiments.

## CONCLUSION

We have illustrated a series of applications of the Monte Carlo method to process and device simulation. The technique provides a very useful tool for the understanding of the physical phenomena and is becoming a fundamental aspect in the area of CAD.

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