# Modeling of Impact Ionization in a Quasi Deterministic 3D Particle Dynamics Semiconductor Device Simulation Program[1]

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## Abstract

A *first principle based quasi-deterministic 3D particle dynamics Monte Carlo simulation* method was developed for examining mesoscopic (subhalf–micron) Si electron devices. Applying a *novel method for calculating the field and potential distributions*, the real trajectories of the carriers are exactly followed. Consequently, an important feature of this method is that *all Coulomb scattering* are inherently taken into account. A brief description of the *physical background*, the *models* and the *simulation principle* is given. A quasi deterministic model for *impact ionization* is developed and some *results* are presented.

## 1. Introduction

Assuming a Si device structure with a volume of $0.25 \times 0.25 \times 0.25\ \mu m^3$ and a doping density of $10^{23}\ m^{-3}$, the number of ionized impurities is only about $10^3$. The number of carriers is of the same order of magnitude.

The classical methods of semiconductor device simulation (based on the *drift-diffusion* or *hydrodynamic semiconductor equations*) use a *continuum view* and apply certain statistical considerations for the *carrier distribution functions*[2]. The potential distribution is determined by the solution of the *Poisson equation*, requiring a 3D spatial discretization resulting in 10 to 50 thousand elementary cells (ie. the average number of carriers is 1/cell or less). These methods are not valid any more if the number of carriers in the simulated structure, like in this case, lies only in the order of magnitude of a few thousands or less.

The small number of carriers suggested the development of a particle dynamics 3D Monte Carlo simulation method[3], for studying mesoscopic device behaviour, where *the trajectories of each carrier are individually and exactly followed* both in the real space and in the **k**-space (wave vector space). The simulation of 3D structures is sometimes simplified to a 2D approach. This simplification cannot be applied for the particle dynamics Monte Carlo simulation of

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[2] Derived from the Boltzmann transport equation (applying the relaxation time approximation and considering the first few momenta of the electron distribution function).

[3] In particle dynamics, all charged particles - i.e. charged carriers, dopant ions, interface charges - are treated as point charges, with no charge assignment to elementary volumes. More sophisticated Monte Carlo methods (by applying charge clouds, superparticles etc.) can offer far more effective numerical solution tools, but the physics of the simulated system can easily be obscured.

charged particles[4]. However, real 3D effects, such as impact ionization or ionization by α particles can not be properly examined by 2D simulations.

## 2. Principle of simulation

Our 3D particle dynamics Monte Carlo semiconductor device simulator program,MicroMOS has been developed for examining sub-half micron silicon MOS transistors andis based on the *concepts of classical physics* (Newton law, Coulomb law, etc.). During development, the attention was focused to apply the deepest possible *first physical principles* inside the examined structure. The elementary particle nature of the carriers is only taken into consideration by anizotropic effective masses, and by Bragg reflection based limitations in their momenta (velocities). Thus all carriers remain in the first Brillouin zone. In this way, the bulk behaviour can be modeled quite accurately. However, near the Si-$SiO_2$ interface the *wave nature of the carriers* must be taken into consideration[5]. For a more detailed description of this method see [1], [2].

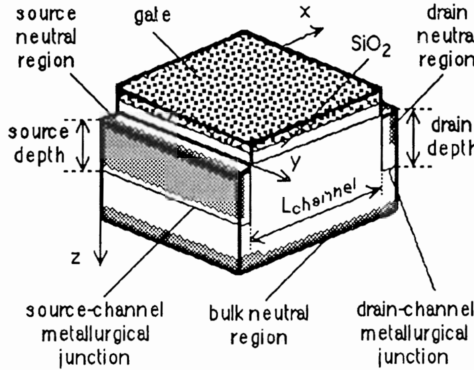


Fig. 1.: The examined MOS structure

The *state of carriers* is characterized by the space coordinate vector **r** and by the wave vector **k**.

The *carrier dynamics* is described by the Newton law

$$\mathbf{a} = m_{\mathrm{eff}}^{-1} \cdot \mathbf{F} \quad (1)$$

where $m_{\mathrm{eff}}^{-1}$ is the *reciprocal effective mass tensor.*

Different transverse and longitudinal effective masses are used. Both masses are considered to be energy independent, resulting in the well known 6 ellipsoidal constant energy surfaces in the **k**-space for electrons. Different izotropic (scalar) effective masses are considered for the light and heavy holes[6], resulting in spherical constant energy surfaces in the **k**-space.

The *forces acting to the carriers* are splitted into two components:

- *the Coulomb force originating from charges inside the structure* (donors, acceptors and charged interface states), evaluated by the Coulomb law.
- *the force caused by the field of external voltages* is evaluated by a boundary value problem solution of the Laplace equation[7].

The first integral of Eq.1 yields the new carrier velocities, the second one the new real space position coordinates[8]. Initial values of the integrations are the carrier position and velocity results of the previous simulation step. To preserve neutrality, at the beginning of each simulation step electrons and holes are injected into predefined source and drain neutral regions. A similar neutral region exists deep in the bulk. Any carriers leaving the structure are annihilated at the end of each simulation step.

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4 The *point charges* in 2 dimensions can only be implemented as *line charges*. In this case we would get an electric field of $1/r$ dependence and a potential of logarithmic dependence, instead of the $1/r^2$ and $1/r$ behaviours, respectively. Since the force acting to the charged carriers is proportional to the field, the calculated trajectories would be sufficiently different from the real 3D ones in any 2D case.

5 The quasi 2D nature of electrons is taken into consideration by the triangular potential well approximation. The electrons are positioned at the first momenta of their wave function. The first 3 subbands are considered.

6 The split-off holes are not taken into consideration.

7 With modified boundary conditions, compared to the usual solution of the Poisson equation.

8 The lowest order numerical integration formulae are used, because the force is a strongly varying function of the space coordinates, therefore using a higher order formula will not give any accuracy improvement. On the contrary, it is possible that the result will be less accurate.

The advantage of this method is that any *Coulomb scattering process* (carrier - ionized impurity, carrier - carrier and carrier - interface state) is exactly followed in a deterministic way[9].

The *interactions between the carriers and the lattice* are described by Bragg scattering mechanisms: if a carrier leaves the first Brillouin zone, it is scattered back to the same Brillouin zone. For the shape of the Brillouin zone the Debye approximation is used[10]. Near the Si-$SiO_2$ interface f- and g- phonon *intervalley scattering processes* are taken into consideration.

*Impact ionization* takes place if the kinetic energy of a carrier exceeds the *impact ionization threshold energy* (for silicon $W_{th}$= 1.8 eV, according to set 1 of [3]). When a carrier has an energy of $W > W_{th}$, a new electron-hole pair is generated. It is assumed, that the ionizing particle looses its whole kinetic energy, and an energy equal to the band gap energy $W_G$ is transferred to the lattice. The momentum and energy conservation conditions are fulfilled for the event. For the *Auger recombination* a phenomenological approach is used, based on a scattering cross section concept: a recombination event occurs, when the distance sinks below a critical distance between a single electron and a hole.

At the Si-$SiO_2$ interface random *elastic and specular surface scattering events* are simulated[11].

## 3. Results and discussion

Table 1. shows geometrical dimensions, doping concentrations, interface charge density and the operating point of the examined MOS transistor, together with physical parameters of the simulation. The simulation time step was $\Delta t = 0.01$ ps. The transistor is in an unsaturated operating point, $I_D \approx 17.3\,\mu A$. Fig. 2. shows the spatial electron distribution in the structure. It can be observed that the electrons near the silicon surface are grouped into subbands. In the followings, we summarize some results related to impact ionization during a 2 ps time interval. Table 2. shows the drain current $I_D$ and impact ionization rates S, giving a detailed picture on the contribution of electrons corresponding to the different constant energy ellipsoid orientations. Observe, that the <100> electrons have a negative contribution to the current, because their positive x-velocity is limited by the maximum value of the corresponding wave vector (0.16 $k_{Max}$). Fig.3. gives the spatial distribution of the impact ionization events, caused by electrons corresponding to various constant energy ellipsoid orientations. On Fig. 4, the impact ionization rate is shown along the x-axis. Fig. 5. shows the energy distribution of the ionizing electrons.

Table 1.

| Parameter | Symbol | Value | Unit |
|---|---|---|---|
| Channel length | L | = 250 | nm |
| Source length (x direction) | $L_S$ | = 30 | nm |
| Drain length (x direction) | $L_D$ | = 33 | nm |
| Source and drain depth | $D_{S,D}$ | = 120 | nm |
| Length of structure | L | = 323 | nm |
| Depth of structure | D | = 302 | nm |
| Width of structure | W | = 259 | nm |
| Gate oxid thickness | $d_{ox}$ | = 4.5 | nm |
| Channel and bulk doping concentration | $N_A$ | = $10^{23}$ | $m^{-3}$ |
| Source and drain doping concentration | $N_D$ | = $10^{24}$ | $m^{-3}$ |
| Charged interface state density | $N_{SS}$ | = $-10^{16}$ | $m^{-2}$ |
| Gate material | Al | | |
| Fuchs parameter | F | = 0.5 | |
| Impact threshold energy | $W_{TH}$ | = 1.800 | eV |
| Auger coefficient | $B_n$ | = 3.5 $10^{-42}$ | $m^6/s$ |
| Drain - source voltage | $U_{DS}$ | = 0.5 | V |
| Gate - source voltage | $U_{GS}$ | = 3.0 | V |

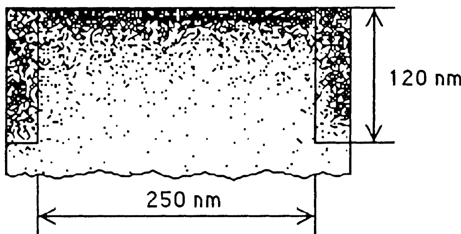


Fig. 2.: Spatial electron distribution

[9] Assuming that the time step $\Delta t$ is small enough.
[10] The dodecaeder shaped first Brillouin zone is approximated by a sphere.
[11] The ratio of these events controlled in order to maintain an average ratio determined by the Fuchs parameter.

Table 2.

| | <001> | <00$\bar{1}$> | <010> | <0$\bar{1}$0> | <100> | <$\bar{1}$00> | Σ |
|---|---|---|---|---|---|---|---|
| $I_D$ [μA] | -19.6 | 18.4 | 1.8 | 5.7 | 3.8 | 7.2 | 17,3 |
| S [1/ps] | 0.47 | 0.44 | 0.64 | 0.60 | 0.17 | 0.28 | 2.60 |

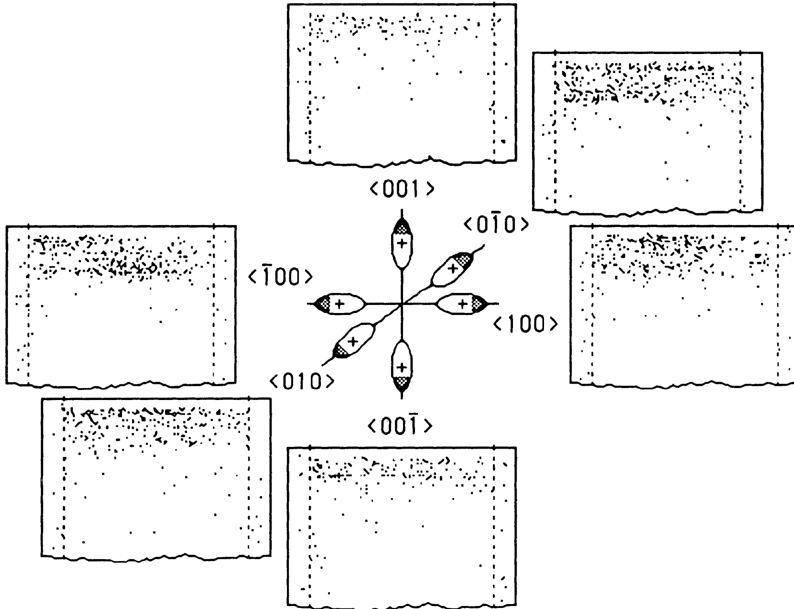


Fig. 3. Spatial distribution of impact ionization events

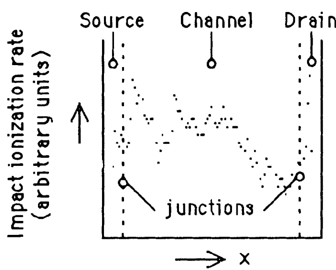


Fig. 4.: Impact ionization rate along the channel

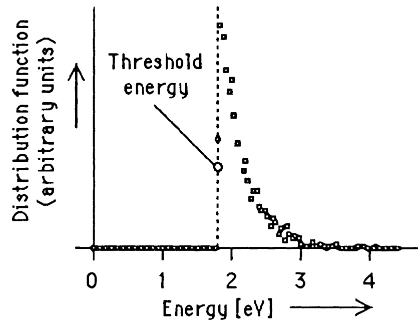


Fig. 5.: Energy distribution of ionizing electrons

## References

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