Accurate Monte Carlo Modeling of Terminal Currents in Short Semiconductor Devices by Using a Generalized Ramo-Shockley Theorem

P. Houlet, Y. Awano, N. Yokoyama and C. Hamaguchi[1]

Fujitsu Laboratories Ltd.
10-1 Morinosato-Wakamiya, Atsugi 243-0197, Japan
Phone +81-462-508247, Fax +81-462-508844,
Email houlet@qed.flab.fujitsu.co.jp

[1]Department of Electronic Engineering
Osaka Unversity, 2-1 Yamada-oka, Suita, Osaka 565-0871, Japan

1. Introduction

The exponential trend of scaling down of semiconductor devices requires a deep continued effort for processing devices into the deep submicron range. The cost for processing such devices is also increasing rapidly and thus acts as a brake upon developing new technologies of which performances and limits are not clearly stated. At this level, the simulation tool plays a fundamental role for predicting performance gains as well as peculiar advantages and shortcomings.

To date the most comprehensive techniques for modeling transport and operation of submicron semiconductor devices are based on numerical solutions of the Boltzmann equation. Among them, the Monte Carlo method has emerged to be a powerful technique because it is closed to the corpuscular reality, without approximations in solving the Boltzmann equation and takes naturally into account hot-carrier and transient phenomena. However, due to its stochastic nature and the finite number of simulated particles, the Monte Carlo method meets with difficulties in calculating quantities on a hydrodynamic time scale such as the transient and average energy, velocity, etc., and also currents measured in the output circuit, in particular in the subthreshold regime. Moreover, device performances in ULSI technologies are very sensitive to phenomena such as dopant fluctuations, process oriented noise, quantum fluctuations, etc., which require for their study to make an great effort on reducing the noise due to the computer simulation techniques.

In this communication, we present an efficient and simple method using a generalized formulation of the Ramo-Shockley theorem for the calculation of the time-dependent terminal currents in multi-port devices within the ensemble Monte Carlo modeling, including the displacement current and the separate contribution of each particle type. Moreover, our technique is optimised for the cloud-in-cell and box-integration framework. We emphasize that our formulation does not require any additional optimization theory, is easy to implement and does not increase CPU time consumption.

2. Generalized Ramo-Shockley theorem

The well-known Ramo-Shockley theorem [1,2] states the total steady-state conduction current flowing through the contact k of a multiport device as

$$I_k = \sum_n q_n \mathbf{W}_k(\mathbf{r}_n) \cdot \mathbf{v}_n \qquad (1)$$

where n is the particle number, q its charge, $\mathbf{r}$ and $\mathbf{v}$ its position and velocity vectors respectively. $\mathbf{W}_k$ is the electric field vector obtained when all charges have been removed from the domain and all contacts grounded except for contact k biased at 1 V. This theorem has been successfully implemented in 1D structures and two-port devices [3], and three-port devices making use of test-function optimiza-

0-7803-4369-7/98 $10.00

tion method [4]. Although this theorem assumes a constant applied bias condition in time and homogeneous material, it has been extended to inhomogeneous media (materials with different dielectric constants) [5] and time dependent contact bias [6]. Then the generalized Ramo-Shockley theorem takes the following formulation

$$I_k(t) = \sum_n q_n \mathbf{W}_k(\mathbf{r}_n(t)) \cdot \mathbf{v}_n(t) \quad (2)$$

This formulation gives the instantaneous total conduction current at any contact of a multiport device with any structure shape. Note that this theorem, by using all the simulated particles, allows to optimize the reduction of the statistical fluctuations caused by the particle discretisation, since in general fluctuations are inverse proportionnal to the particle number. Note also that $\mathbf{W}_k$ is an unvariable geometrical factor which is related to the structure of the device. For a 1D structure of length L, $\mathbf{W}_k$ takes the uniform value of $1/L$, and the Ramo-Shockley theorem reads

$$I(t) = \frac{1}{L} \sum_n q_n v_n(t) \quad (3)$$

where v_n is the carrier velocity along the device orientation.

3. Accurate current estimator

The total conduction current contains the electron and hole contributions as

$$I_c(t) = I_e(t) + I_h(t) \quad (4)$$

where I_e and I_h are the electron and hole conduction currents respectively, which can be calculated independently using Eq. 2 as

$$I_{c,k}(t) = \sum_n q_{e,n} \mathbf{W}_k(\mathbf{r}_{e,n}(t)) \cdot \mathbf{v}_{e,n}(t) \quad (5)$$

$$I_{h,k}(t) = \sum_n q_{h,n} \mathbf{W}_k(\mathbf{r}_{h,n}(t)) \cdot \mathbf{v}_{h,n}(t) \quad (6)$$

with subscript e and h standing for electrons and holes, respectively.

When the contact bias are varying in time we have to add the displacement current $I_{d,k}$ to the conduction current $I_{c,k}$ to obtain the total current $I_{t,k}$ such as

$$I_{t,k}(t) = I_{c,k}(t) + I_{d,k}(t) \quad (7)$$

To reduce statistical errors, the cloud-in-cell and box-integration methods [7,8] can be used within the Monte Carlo scheme. Thus we can also apply these method to the current calculations to further improve accuracy. Since the electric field and the charge are discretized at the grid points of a non-uniform tensor product grid, the particle velocity in Eq. (2) has also to be discretized in the same way for consistency. This means the velocity of the charge at the grid points has to be calculated instead of the particle velocity. In this case, we obtain the conduction current at the grid point ij

$$I_k(t+T) = \frac{1}{T} \sum_{ij} (Q_{ij}(t+T) - Q_{ij}(t)) \mathbf{W}_{k,ij} \cdot \mathbf{b}_{ij} \quad (8)$$

where Q_{ij} is the nodal charge, T the duration timestep and $\mathbf{b}_{ij}$ is the vector defining the box at the grid point ij.

The displacement current can be calculated from the current density

$$\mathbf{j}_d = \varepsilon \frac{\partial \mathbf{E}}{\partial t} \quad (9)$$

and by integrating it over the contact section, for example, as in Ref. [9].

So we have calculated both conduction and displacement currents with a high accuracy using separate computations. Our method is applicable to any kind of structure, at any bias conditions and in particular in subthreshold regime due to the use of all simulated particles which allows to ultimately reduce computational noise. We can notice also that our method generalizes the original results of [10] (See Eq. 16 to 18 of [10]) which gives a 1D approximation of the conduction currents for specific structure shapes. We can easily show for example that Eq. 16 of [10] is a 1D approximation of our Eq. 7 where contacts have been placed at x_s and x_{g1}, according to the notations of [10].

4. Results and conclusions

We present apllications of our method to the case of HEMT and MOSFET devices. On figure 1 is reported the structure of the simulated AlGaAs/GaAs

0.3 μm gate length HEMT. Doping densities are 10^{18} cm^{-3} near contacting area and 10^{16} cm^{-3} in the channel. The model includes 3D electrons in the channel, as well as 2D electrons up to the pinch-off point, and the real space transfert. Results of the instantaneous steady-state drain current are reported on figure 2 with our method and the standard particle-counting method at the contact. Let's notice that the current calculated at the contact takes discrete values corresponding to the number of particles counted at each sample time. To obtain continuous data, it is necessary to cumulate data over the time. On figure 3 we have reported the structure of the simulated 0.13 μm gate-length n-MOSFET. Doping densities are 2×10^{20} cm^{-3} near contacting area and 10^{16} cm^{-3} in the channel. Cumulated steady-state drain-current calculated with our method and by particle counting at the contact are reported on figure 4. One shall notice that we obtain excellent accuracy although the high doping used in the contacting regions (2×10^{20} cm^{-3}). We notice also that by using the particle counting at contact the convergence is difficult to obtain. This is enhanced by the specific shape for the source and drain electrodes we have used in our structure modelling.

In conclusion, we have presented an efficient and simple method to evaluate terminal currents in semiconductor devices, based on a generalized formulation of the Ramo-Shockley theorem. Moreover, our method takes advantage of the cloud-in-cell and box-integration techniques.

References

1. W. Shockley: J. Appl. Phys. **9** (1938) 635.
2. S. Ramo: Proc. IRE **27** (1939) 584.
3. L. Varani and L. Reggiani: Rivista del Nuovo Cimento 17, **7** (1994), and references therein.
4. P.D. Yoder, K. Gärtner, U. Krumbein and W. Fichtner: IEEE Trans. on CAD **10** (1997) 1082.
5. P. De Visschere: Solid Stat. Electron. **33** (1990) 455.
6. H. Kim, H. S. Min, T. W. Tang and Y. J. Park: Solid Stat. Electron. **34** (1991) 1251.
7. R. W. Hockney and J. W. Eastwood, *Computer Simulation Using Particles* (Institute of Physics Publishing, Bristol, Philadelphia, 1988)
8. M.V. Fischetti and S. E. Laux: Phys. Rev. B **38** (1988) 9721.
9. P. Graf, S. Keith and B. Meinerzhagen, *SISPAD '97* (1997).
10. V. Gruzhinskis, S. Kershulis and A. Reklaitis: Semicond. Sci. Technol. **6** (1991) 602.

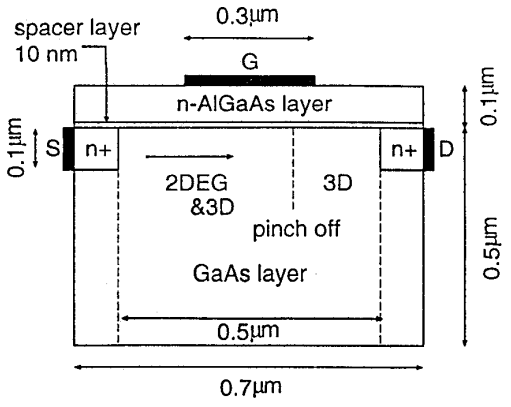

Figure 1: Structure of the simulated HEMT

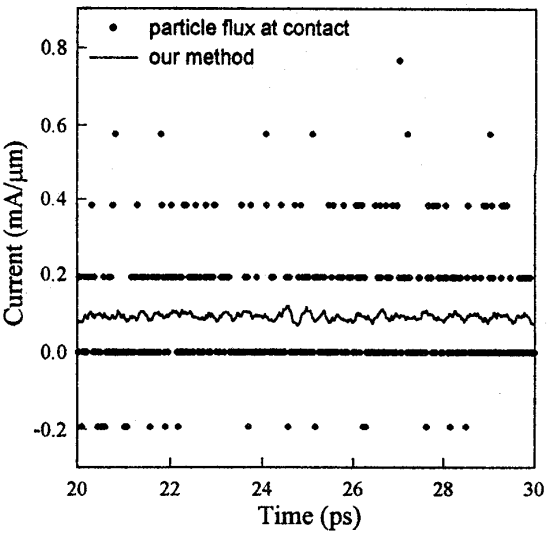

Figure 2: Instantaneous drain current for $V_{DS} = 0.8$ V and $V_{GS} = 0.1$ V in the steady-state regime of the HEMT. Plotted data are sampled each 30fs. The current calculated at the contact takes discrete values corresponding to the number of particles counted at each sample time.

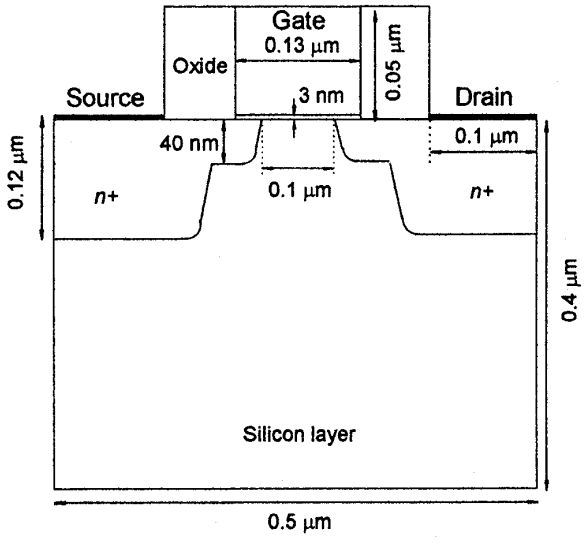

Figure 3: Structure of the simulated MOSFET

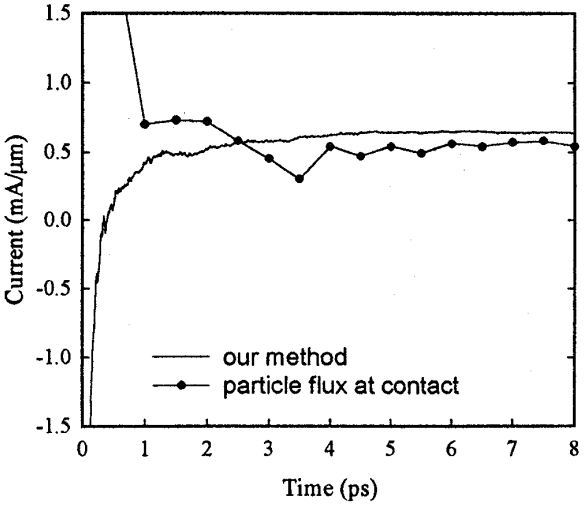

Figure 4: Cumulated drain current in the steady-state regime for $V_{DS} = 2$ V and $V_{GS} = 1.5$ V in the steady-state regime of the MOSFET. Data are cumulated during 0.5ps for particle counting at contact and for 0.005ps for our method.