Solid-State Electronics 84 (2013) 112–119

Contents lists available at SciVerse ScienceDirect

Solid-State Electronics

journal homepage: www.elsevier.com/locate/sse

Deterministic solvers for the Boltzmann transport equation of 3D and quasi-2D electron and hole systems in SiGe devices ☆

C. Jungemann [a,*], A.-T. Pham [b], S.-M. Hong [c], L. Smith [b], B. Meinerzhagen [d]

[a] ITHE, RWTH Aachen University, 52056 Aachen, Germany
[b] Synopsys Inc., 700 E Middlefield Rd., Mountain View, CA 94043, USA
[c] School of Information and Communications, Gwangju Institute of Science and Technology, Gwangju 500-712, Korea
[d] BST, TU Braunschweig, Postfach 3329, 38023 Braunschweig, Germany

ARTICLE INFO

Article history:
Available online 12 March 2013

Keywords:
Boltzmann transport equation
Schrödinger equation
Deterministic solvers
Spherical harmonics expansion
Silicon
Non-symmetric operator ordering

ABSTRACT

We present a review of recent advances in deterministic solvers for the Boltzmann transport equation for electrons and holes in a 3D and quasi 2D $\vec{k}$-space and demonstrate the capabilities of deterministic solvers by two new examples: a THz SiGe HBT and a quantum well PMOSFET. Compared to the standard approach, the Monte Carlo method, these deterministic solvers have certain advantages. They yield exact stationary solutions and they allow small-signal and noise analysis directly in the frequency range from 0 to THz. Inclusion of magnetic fields, the Pauli principle or rare events causes no problems. Thus, it is now possible to calculate certain key figures of merit for devices based on the Boltzmann transport equation, which was previously very difficult or not possible at all. On the other hand, the deterministic solvers are more memory intensive and more difficult to code than the Monte Carlo method.

1. Introduction

The Monte Carlo (MC) method is the standard approach to solve the Boltzmann transport equation (BTE), which describes transport of electrons and holes in the semi-classical framework (e.g. [2]). The MC method itself is a numerical approach to integration and its accuracy is inversely proportional to the square root of the CPU time (e.g. [3]). In the case of the BTE the MC solver is inherently transient and the solution contains stochastic noise. If the physical MC approach is used, the stochastic noise is proportional to the physical noise of the carriers (e.g. [4]). The usual MC method for devices is charge conserving and in the case of sufficiently short time steps for the self-consistent solution with the Poisson equation relatively stable (e.g. [5]). The MC method is well understood and easy to code. Complex microscopic models can be included (e.g. full bands [6]). Due to its many advantages the MC approach is the method of choice for the solution of the BTE and frequently used.

On the other hand, problems arise for example, when the MC method is applied to processes, which are rare or evolve on a relatively long time scale. A typical example is the floating body effect in SOI devices, where rare events (impact ionization or tunneling) lead to hysteresis effects in the millisecond range and low-frequency noise [7]. By now no successful simulation of this problem with an MC method has been demonstrated. Self-consistent MC device simulations require time step lengths in the order of femtoseconds to resolve the plasma oscillations [8] and simulations for milliseconds are not feasible. Even simulation times of nanoseconds are not feasible and the RF behavior of transistors at technically relevant frequencies (i.e. in the lower GHz range) cannot be simulated by MC (see discussion in Ref. [9]). Furthermore, small-signal behavior is difficult to simulate, since no small-signal MC approach for devices is known and double randomization has to be used with its unfavorable stochastic properties. This makes it very difficult to calculate key figures of merit for RF transistors (e.g. cutoff frequency). Even standard stationary MC device simulations might require excessive CPU times [10]. Inclusion of the Pauli principle is possible [11], but requires in devices rather larger particle ensembles and restricts the simulations to relatively short durations of simulated time [12].

The shortcomings of the MC method have led to a search for alternative methods and the most successful one is the deterministic spherical harmonics expansion (SHE), which was used already in the earliest days of solving the BTE (e.g. [13]). In devices not only the $\vec{k}$-space but also the real space has to be discretized resulting in huge memory requirements, and for a long time device simulations by SHE were not possible or required very expensive super computers in contrast to MC. In recent years this problem has been

☆ This article is an extended version of a paper presented at ESSDERC 2012 [1].

* Corresponding author.
E-mail address: cj@ithe.rwth-aachen.de (C. Jungemann).

0038-1101/$ - see front matter © 2013 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.sse.2013.02.034

aleviated by advances in DRAM technology and today computers with more than 100 GBytes are readily available removing the main obstacle.

In the case of a quantized system (e.g. the channel of a MOSFET) the $\vec{k}$-space is 2D and instead of SHE a Fourier harmonics expansion (FHE) of the polar angle is used [14,15]. Otherwise the same methods can be applied as in the case of SHE [16].

In this paper recent developments of the SHE method are reviewed. The method is introduced in the next section and in the following sections two new examples of challenging device simulations are presented. The first example is a THz SiGe HBT, for which the characterization includes low currents, breakdown voltages, AC and noise behavior, all of which are difficult to calculate by the MC method. In the second example a quantum well PMOSFET is investigated, where the FHE approach enables the self-consistent solution of the Poisson equation together with the Schrödinger equation based on a complex Hamiltonian without further approximations in contrast to previous approaches (e.g. [17]). Further examples of various device simulations by SHE and FHE can be found in Ref. [16].

2. Spherical harmonics expansion

In order to reduce the number of dimensions of the problem, the distribution function in the 3D $\vec{k}$-space is expanded with spherical harmonics based on spherical coordinates w.r.t. the angles [18,19]. Spherical harmonics are used for this expansion in the hope that they capture the symmetry of the problem and thus converge quickly leading to a small $l_{\max}$

$$f(\vec{k},\vec{r}) = f(\varepsilon,\vartheta,\varphi,\vec{r}) \approx \sum_{l=0}^{l_{\max}} \sum_{m=-l}^{m=l} f_{l,m}(\varepsilon,\vec{r}) Y_{l,m}(\vartheta,\varphi), \quad (1)$$

where $\vec{k}$ is the wave vector, $\vec{r}$ the position in real space, ε the energy, ϑ,φ the spherical angles in the $\vec{k}$-space, $Y_{l,m}$ the spherical harmonics and $l_{\max}$ the maximum order of the SHE. This leads to a projection of the BTE which results in balance equations for the coefficients of the expanded distribution function in energy and real space. Thus, the number of dimensions of the solution domain is reduced by two at the cost of multiple and coupled balance equations. These balance equations can be handled with numerical methods similar to the drift–diffusion model (finite volume method, dimensional splitting, etc.) [20,16] and easily integrated in a standard TCAD framework. The initial problems with numerical stability have been successfully solved (e.g. H-transform [18], maximum entropy dissipation scheme [21,20], for details see [16]). With this approach stationary self-consistent solutions of the BTE and Poisson equation can be calculated for devices, where the final convergence is ensured by the Newton–Raphson method [22], even in the case where the Pauli principle is considered [23]. In addition, exact small-signal and noise analysis is possible directly in the frequency domain [24,16]. This led to the first simulations of partially depleted SOI-NMOSFETs including the kink-effect and noise based on the BTE [16]. Cyclostationary simulations with the harmonic balance approach are possible [25]. Full-band structures can be included with different levels of approximation [26,27,16]. Exact inclusion of full-bands is possible [20], if the relation between energy and the modulus of the wave vector is monotonic [28]. Bipolar device simulations by SHE of electrons and holes together with generation/recombination processes have been demonstrated [29]. Magnetic fields can be included and the small changes in transport can be accurately calculated [30]. Even quantum transport effects have been considered [31].

About 80 GBytes of memory are required for a DC and small-signal simulation of a device, which is 2D in real space. Although memories of this size are available today, a method has been developed to reduce the memory requirements [32], and a DC simulation of a FinFET, which is 3D in real space, has been demonstrated recently, where the memory requirement was less than 12 GBytes [33]. The simulation is based on a tetrahedral grid in real space and an adaptive maximum SHE order in the energy/real space.

3. SiGe HBT

The first example is the THz SiGe HBT of Ref. [34], which is simulated with a box and a drift Ge profile. The vertical doping and Ge profiles are shown in Fig. 1. Both Ge profiles have the same total Ge content. The drift profile is non-standard, because it extends into the highly-doped emitter. The maximum concentrations of donors and acceptors exceed $10^{20}/\mathrm{cm}^3$. The 2D geometry is shown in Fig. 2. It is assumed that the transistor is symmetric to the line $y = 0$ and the width of the emitter window is 2×25 nm. The simulation grid in the real space is indicated by the ticks in Fig. 2. It has 120 lines in x-direction and 20 in y-direction resulting in 2400 grid nodes in real space. The spacing of the H-grid is 5.167 meV. The total number of variables depends on the maximum order of the SHE and the applied bias conditions, which determine the range of the H-grid. In the case of small-signal or noise analysis complex numbers are used and the memory requirement doubles. The noise simulations shown in Fig. 8 required about 80 GBytes of memory. The CPU time for the DC simulations shown in Fig. 5 was about 5 h per bias point on a current computer.

The SHE solver is initialized with a potential calculated by a consistent drift–diffusion model. Then a few Gummel-type relaxation steps are used to reduce the error in the potential further. Below a certain threshold the Newton–Raphson iteration, which solves the Poisson equation and BTE self-consistently, is started [16]. Its convergence is demonstrated in Fig. 3. Within five iterations the Newton–Raphson method is converged (potential corrections lower than 10^{-10} V). The rapid superlinear convergence indicates that the solution is very close to the real solution of the system of nonlinear equations and reliable. In addition, an exactly stationary solution is obtained in contrast to the transient MC method [8]. The electron density is shown for the drift transistor in Fig. 4 at a very low base/emitter bias of 0.4 V. In this case the density varies by 15 orders of magnitude. Nevertheless, a stable solution is obtained and no spurious oscillations occur. This demonstrates the extraordinary numerical stability of the H-transform in conjunction with maximum entropy dissipation scheme. Huge variations in density cause no problems, whereas in the case of the MC method simulation of low densities is only possible by

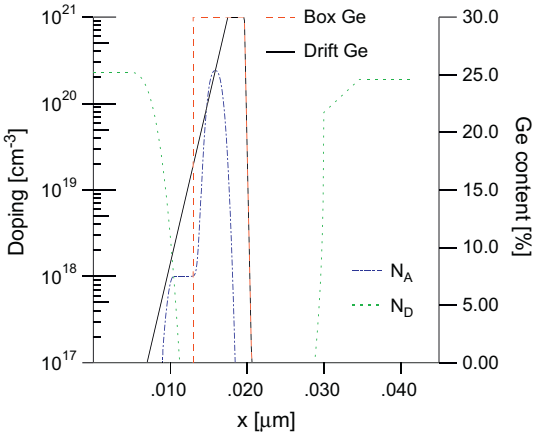

Fig. 1. Doping and Ge profiles of the SiGe HBT.