Full-Band Monte Carlo Device Simulation of a Si/SiGe-HBT with a Realistic Ge Profile

S. Keith, C. Jungemann, S. Decker, B. Neinhüs, M. Bartels and B. Meinerzhagen
Institut für Theoretische Elektrotechnik und Mikroelektronik
Universität Bremen, Kufsteiner Straße, Postfach 33 04 40, 28334 Bremen, Germany
Tel.: +49 421 218 2204, Fax: +49 421 218 4434

Abstract

In this paper we present full-band Monte Carlo simulations of an advanced Silicon/Silicon-Germanium Heterojunction Bipolar Transistor. In addition to this 2D MC simulations we performed simulations with a 1D MC model and a hydrodynamic model. For main internal distributions good consistency is found. We conclude with a microscopic investigation of the full-band Monte Carlo results.

1 Introduction

Silicon/Silicon-Germanium Heterojunction Bipolar Transistors (HBT) are promising devices for low-cost high frequency applications in mobile communication. Hence, there is an increasing demand for an accurate modeling of SiGe heterodevices. The solution of Boltzmann's transport equation by means of the full-band Monte Carlo method (FB-MC) relies only on few simplifications of carrier transport physics. Thus, this method is expected to describe device behaviour of heterodevices reliable and can be used to validate classical simulators that are based on macroscopic transport equations. The transport coefficients of our hydrodynamic model (HD) are extracted from homogeneous FB-MC simulations to ensure consistency [1, 2]. The 2D HBT test structure is derived from an advanced HBT from an industrial pilot line process with a realistic Ge-profile [3, 4, 5].

2 Simulation method

The FB-MC code is based on the scattering models reported in [6] with optical phonons and acoustic phonons in the isotropic and elastic equipartition approximation. In SiGe the phonon scattering mechanisms are approximated by considering both Si and Ge phonons and weighting the respective scattering rate by the relative fraction of the component in the alloy. Furthermore alloy scattering is modeled analogous to [7]. Scattering by ionized impurities is taken into account including a doping dependent adjustment to match experimental minority and majority mobility data. The band structures are calculated with the nonlocal empirical pseudopotential method [8]. The valence and conduction bands are discretized in k-space with nonuniform unstructured grids which minimize the discretization error [9]. Bandgap narrowing due to the doping is considered by the traditional model of [10] with the parameters given in [11]. N_T is the total doping.

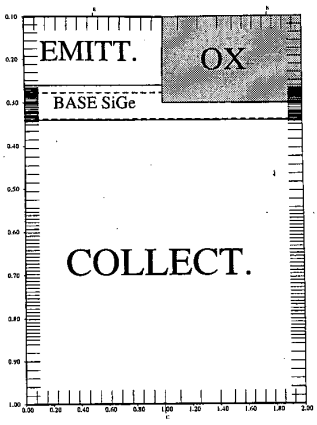

Fig. 1: The 2D SiGe-HBT test structure

$$\Delta E_{bgn} = E_0 \left(\ln \frac{N_T}{N_{Ref}} + \sqrt{\left(\ln \frac{N_T}{N_{Ref}} \right)^2 + 0{,}5} \right)$$

with $E_0 = 0{,}009\,eV$, $N_{Ref} = 1{,}0 \cdot 10^{17} cm^{-3}$

Band energy shifts depending on the germanium content x_{Ge} are calculated as reported in [11]. The entire band offsets are given below.

$$\Delta E_c = (-0{,}228\, x_{Ge} + 0{,}298\, x_{Ge}^2) eV - \frac{1}{2} \Delta E_{bgn}$$

$$\Delta E_v = (0{,}732\, x_{Ge} + 0{,}098\, x_{Ge}^2) eV + \frac{1}{2} \Delta E_{bgn}$$

In Fig. 1 the 2D SiGe HBT test structure is shown. The maximum acceptor doping is $3 \times 10^{19} cm^{-3}$. The lowly doped emitter and the collector have a donator doping of about $3 \times 10^{18} cm^{-3}$ and $2 \times 10^{16} cm^{-3}$, respectively. In the emitter and collector contact region the maximum donator concentration is limited to $1 \times 10^{19} cm^{-3}$ in order

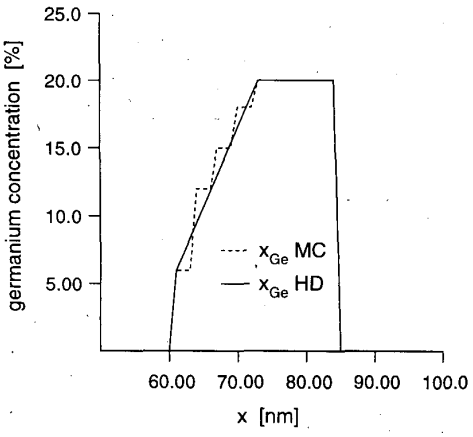

Fig. 2: Germanium profile in the base [3]

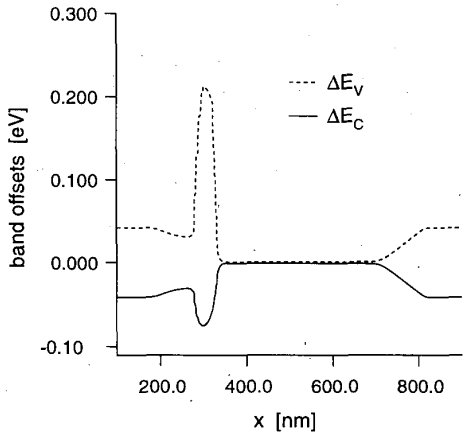

Fig. 3: Band offsets

to reduce the effect of carrier self-heating during the MC simulations. It has been checked by HD simulations that this reduction of the maximum donator doping does not obscure the simulation results in comparison with simulations based on the original doping profile. Arbitrary germanium profiles are resolved spatially in a stepwise manner. The utilized germanium profile is similar to the profile in Fig. 2. The resulting band offsets are shown in Fig. 3, which lead to an energy barrier for electrons passing the emitter/base-junction. Particle transfers via such hetero interfaces are treated consistently with the full-band structure conserving parallel momentum and energy [12].

The profile is approximated for the FB-MC simulation by 6 different germanium concentrations. Although within our FB-MC code any desired number of bandstructures is possible, the number is limited by the available CPU memory. Less than 50 MBytes are required for one band structure and the total for this simulation is about 320 MBytes including the particle data and statistics. The FB-MC model is solved self-consistently with Poisson's equation. The CPU efficiency of the FB-MC model is similar to the one of the analytical MC model described in [13].

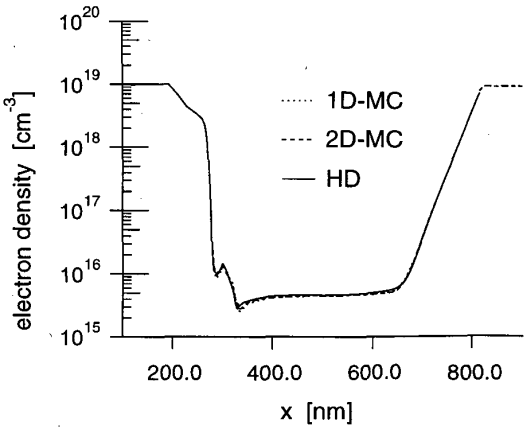

Fig. 4: Comparison of the electron density

3 Results

The results of the HD, 2D MC and 1D MC simulations are summarized in Fig. 4-6 for the electron density, drift velocity and dynamic temperature. In the case of the 1D MC simulation Poisson's equation is solved with a constant hole fermi level. Thereby the CPU times can be reduced in comparison to the 2D-MC model, because no holes have to be simulated and the dimension of the problem is reduced resulting in a smaller number of electrons.

The bias conditions are $V_{BE} = 0.75V$ and $V_{CB} = 2.0V$. The CPU time for $1ps$ with 140.000 particles is 200 minutes for the 2D-MC model on a 300MHz SUN ULTRA 2. The electron density in Fig. 4 shows a good agreement of all three cases. A significant velocity overshoot is found at the base/collector junction for the HD model and for the MC model as well (Fig. 5). The electron temperature in Fig. 6 also shows a good agreement between HD and MC. Only in the base the electron temperature of the 2D MC simulation is slightly raised compared to the other models, because the minority electrons couple strongly with the plasma oscillations of the majority holes. The overall consistency indicates the reliability of the less CPU intensive HD model. The collector current and total CPU time are compared for HD and 1D-MC in Tab. 1. The collector current agrees well within the stochastic error but

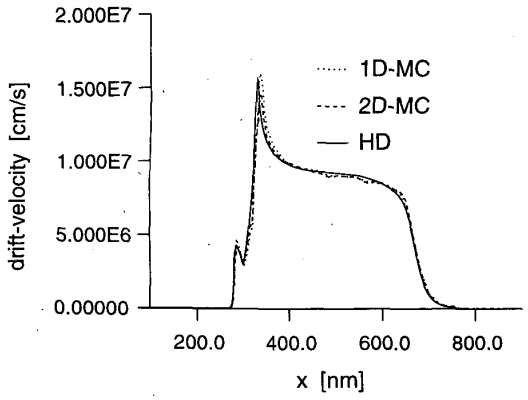

Fig. 5: Comparison of the drift velocity

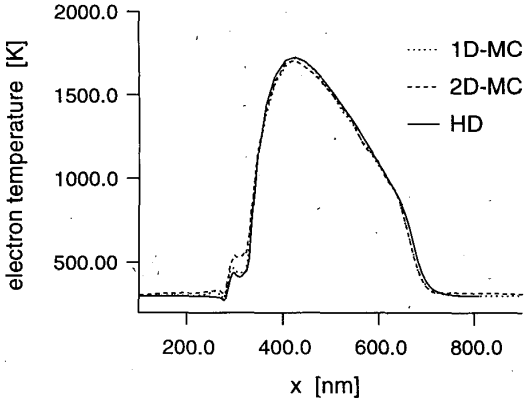

Fig. 6: Comparison of the dynamic temperature

the large difference in CPU time demonstrates the disadvantage of the FB-MC model. The stochastic error in case of the FB-MC simulations is evaluated with the method described in [14]. The calculation is converged with a probability of 95% within ±19%. Additionally the HD simulated GUMMELplot in comparison to measurements of our SiGe HBT test structure is shown in Fig. 7. The good agreement demonstrates the advantages of the fast HD model. For more details concerning the HD simulations see [15].

It is one of the definite advantages of the FB-MC simulation that it enables detailed microscopic investigations, which are impossible by standard HD or DD device models. For example in Fig. 8 the valley occupation of the electrons for the FB-MC simulation is depicted. Due to the biaxial compressive strain in the base the two longitudinal valleys of the first conduction band are shifted upwards in energy, whereas the four transversal valleys are

	HD	1D-MC
I-C	$0.70A/cm$	$0.65A/cm$
CPU-time	40 sec	45 hours
error	–	±19%

Table 1:

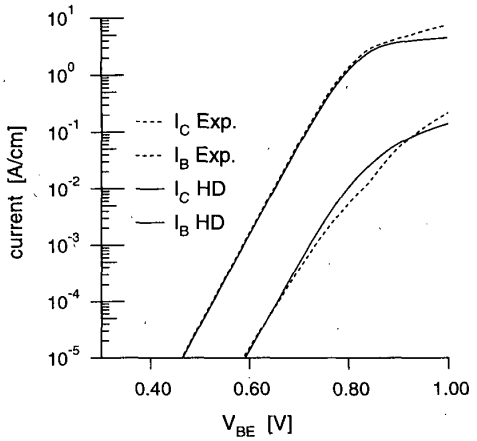

Fig. 7: GUMMELplot at $V_{CB} = 2V$

lowered. Before the base all valleys are uniformly populated, because the electron ensemble is nearly in thermal equilibrium. Since most of the electrons are passing the emitter/base-junction with low energies, the longitudinal valleys are rarely occupied in the base region.

Consequently the transversal-valleys are populated with nearly 25%. In the collector region all six valleys are again equivalent, but the strong electric field increases the population of the longitudinal valleys. In the collector contact the electron gas returns to a state near thermal equilibrium and all valleys are populated by the same number of electrons. Although from a more macroscopic point of view this effect is not important for the test HBT as demonstrated in Fig. 4-6, it might become important for more aggressively scaled devices. Therefore it is very beneficial to have the FB-MC model available for reference simulations. Another important application of the FB-MC model is the examination whether the velocity overshoot in HD simulations is spurious or real. For such investigation the faster 1D-MC model is often sufficient.

4 Conclusion

In conclusion we have reported fully consistent HD and FB-MC simulations of a SiGe HBT with a realistic Ge profile in one and two dimensions. It turns out that the CPU efficient and robust HD model and the MC model

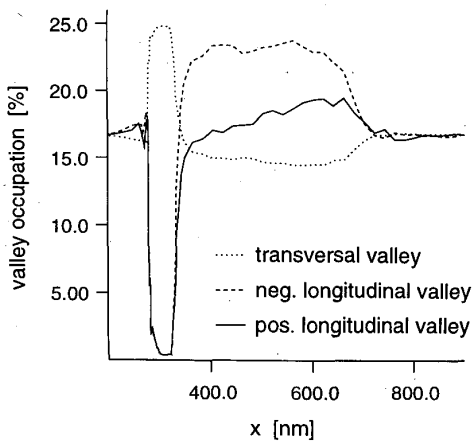

Fig. 8: Valley occupation resulting from MC simulations

agree well for all relevant internal distributions. Therefore, the HD model is currently the best model for the industrial design of SiGe HBTs. The MC model provides more physical insight and is used to validate the accuracy of the HD model.

Acknowledgment

The authors thank A. Schüppen and K. H. Bach of TEMIC Semiconductor GmbH for helpful discussions and providing the experimental data. Partial funding by the Bundesministerium für Bildung, Forschung und Technologie under contract no. 01M2416C is gratefully acknowledged.

References

[1] C. Jungemann, M. Bartels, S. Keith, and B. Meinerzhagen, "Efficient methods for Hall factor and transport coefficient evaluation for electrons and holes in Si and SiGe based on a full-band structure," in *Proc. IWCE*, (Osaka (Japan)), pp. 104–107, 1998.

[2] B. Neinhüs, S. Decker, P. Graf, F. M. Bufler, and B. Meinerzhagen, "Consistent hydrodynamic and Monte–Carlo simulation of SiGe HBTs based on table models for the relaxation times," *VLSI Design*, vol. 8, pp. 387–391, 1998.

[3] A. Schüppen, H. Dietrich, U. Seiler, H. von der Ropp, and U. Erben, "A SiGe RF technology for mobile communication systems," *Microwave Engineering Europe*, vol. June, pp. 39–46, 1998.

[4] A. Schüppen, U. Erben, A. Gruhle, H. Kibbel, and H. Schumacher, "Enhanced SiGe heterojunction bipolar transistor with 160 GHz - f_{max}," in *IEDM Tech. Dig.*, pp. 743–746, 1995.

[5] D. Knoll, B. Heinemann, R. Barth, K. Blum, J.Drews, A. Wolff, P. Schley, D. Bolze, B. Tillack, G. Kissinger, and W. Winkler, "Low cost, 50 GHz Fmax Si/SiGe heterojunction bipolar transistor technology with epi-free collector wells," in *Proc. ESSDERC*, (Bordeaux), pp. 140–143, 1998.

[6] F. M. Bufler, "Full–Band Monte Carlo Simulation of Electrons and Holes in Strained Si and SiGe," Dissertation, Universität Bremen, Bremen, 1997.

[7] J. W. Harrison and J. R. Hauser, "Alloy scattering in ternary III-V compounds," *Phys. Rev. B*, vol. 13, pp. 5347–5350, 1976.

[8] M. M. Rieger and P. Vogl, "Electronic-band parameters in strained $Si_{1-x}Ge_x$ alloys on $Si_{1-y}Ge_y$ substrates," *Phys. Rev. B*, vol. 48, pp. 14276–14287, 1993.

[9] C. Jungemann, S. Keith, M. Bartels, and B. Meinerzhagen, "Efficient full-band Monte Carlo simulation of silicon devices," *IEICE Trans. on Electronics*, vol. E82-C, no. 6, 1999.

[10] J. W. Slotboom and H. C. de Graaf, "Measurements of bandgap narrowing in Si bipolar transistors," *Solid–State Electron.*, vol. 19, pp. 857–862, 1976.

[11] D. Nuernbergk, "Simulation des Transportverhaltens in $Si/Si_{1-x}Ge_x/Si$–Heterobipolartransistoren," Dissertation, Technische Universität Ilmenau, Ilmenau, 1997.

[12] C. Jungemann, S. Keith, and B. Meinerzhagen, "Full-band Monte Carlo simulation of a 0.12μm-Si-PMOSFET with and without a strained SiGe-channel," in *IEDM Tech. Dig.*, (San Francisco (USA)), pp. 897–900, 1998.

[13] P. Graf, F. M. Bufler, B. Meinerzhagen, and C. Jungemann, "A comprehensive SiGe Monte Carlo model for transient 2D simulations of HBTs," in *IEDM Tech. Dig.*, pp. 881–884, 1997.

[14] C. Jungemann, S. Yamaguchi, and H. Goto, "Convergence estimation for stationary ensemble Monte Carlo simulations," *IEEE J. Tech. Comp. Aided Design*, no. 10, 1998.

[15] M. Bartels, S. Decker, B. Neinhüs, K. H. Bach, A. Schüppen, and B. Meinerzhagen, "Comprehensive hydrodynamic simulation of an industrial SiGe heterobipolar transistor," in *Proc. BCTM*, (Minneapolis (Minnesota, USA)), 1999.