# Spatial Analysis of the Electron Transit Time in a Silicon/Germanium Heterojunction Bipolar Transistor by Drift-Diffusion, Hydrodynamic, and Full-Band Monte Carlo Device Simulation

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*Abstract*-**Transit times and cutoff frequency of a silicon/germanium heterojunction bipolar transistor (SiGe HBT) are investigated by consistent drift-diffusion (DD), hydrodynamic (HD), and full-band Monte Carlo (FB-MC) simulations. Good agreement of all three transport models is found for the collector transit time. The quasiballistic transport in the base is well described by the HD model and it yields the same transit time as the FB-MC model, whereas the DD model yields a much larger transit time, because it does not include any velocity overshoot effects at all. Surprisingly, in the emitter region the FB-MC model yields the largest transit time leading to a peak cutoff frequency for the special device structure under investigation which is even smaller than the DD peak value. The strong anisotropy of the strained band structure in the base, which is not captured in full detail by the DD and HD model, is identified as a possible reason for this unexpected behavior.**

## Introduction

The SiGe alloy has made band engineering possible with more or less mainstream Si technologies retaining the cost advantage of Si over III/V materials [1, 2]. Si/SiGe HBTs have been fabricated with a cutoff frequency in the excess of 100GHz [3]. Due to the small base widths of less than 50nm the electron transport becomes more and more ballistic. This calls into question the validity of the standard simulation tools like the DD or HD model used to design high-frequency HBTs. In addition, the strain caused by the pseudomorphic growth of the epilayers results in a strong anisotropy of the band structure only captured in full detail by the FB-MC model.

The impact of the quasiballistic transport and of the anisotropic band structure on the high-frequency properties of an HBT is exemplified in this work by a comparison of DD, HD, and FB-MC simulations for transit times and cutoff frequency. First, the simulation details and then results for an HBT are presented.

## Simulation Details

The details of the FB-MC model can be found in [4, 5]. The band structure is calculated with the nonlocal empirical-pseudopotential method [6] and the conduction-band edge is modeled similar to [1, 7]. The DD and HD model are described in [8], where all transport parameters of the DD and HD model are generated by FB-MC bulk simulations to ensure consistency of the simulation models. In the HD model the heat flux is reduced to 25% as in [9].

With the three simulation models transit times are evaluated for an HBT. In order to reduce the CPU times of the FB-MC simulations a 1D-device approximation is used for the HBT. The missing base contact is simulated by fixing the quasifermi potential of the holes in the center of the base to the value of the base voltage. The 1D-device approximation works well as long as the device is not operated too far in the high-injection regime. In the case of the FB-MC model no holes are simulated and their contribution to the space charge is calculated based on the DD hole quasifermi potential in conjunction with a nonlinear Poisson equation.

In the case of a 1D device approximation the transit time for a region extending from $x_\mathrm{b}$ to $x_\mathrm{e}$ reads [10]

$$\tau(x_\mathrm{b}, x_\mathrm{e}) = \int_{x_\mathrm{b}}^{x_\mathrm{e}} q \left.\frac{dn}{dI_\mathrm{C}}\right|_{U_\mathrm{CE}=\mathrm{const}} dx \tag{1}$$

where $q$ is the electron charge, $n$ the electron density, $I_\mathrm{C}$ the collector current per device area, and $U_\mathrm{CE}$ the collector/emitter voltage. The derivative is calculated by varying the base voltage. The total transit time is inversely proportional to the cutoff frequency: $f_\mathrm{T} = 1/2\pi\tau(0, L)$, where $L$ is the device length [11].

In order to avoid the difficulties of an MC small signal analysis the derivative in (1) is evaluated with the finite-difference technique and in the case of the MC model a change in the base bias of 10mV is used. The small change in the base voltage necessary to avoid nonlinear effects entails MC results with a very low noise level. To this end, the MC simulations are performed until the relative error of the collector current is below 1.0% with a probability of 95.5%. In addition, the statistics are enhanced in regions with low electron densities [4].

## Results

In Fig. 1 the doping profile and the graded Ge profile of the investigated HBT are shown. The maximum donor concentration was limited to $10^{19}/\mathrm{cm}^3$ to improve the time stability of the self-consistent MC device simulations [12]. It was checked by HD simulations that the reduction of the maximum donor concentration does not impair the results of the investigations described below.

The electron density and drift velocity are shown in Figs. 2 and 3, respectively. Quasiballistic transport occurs in the base

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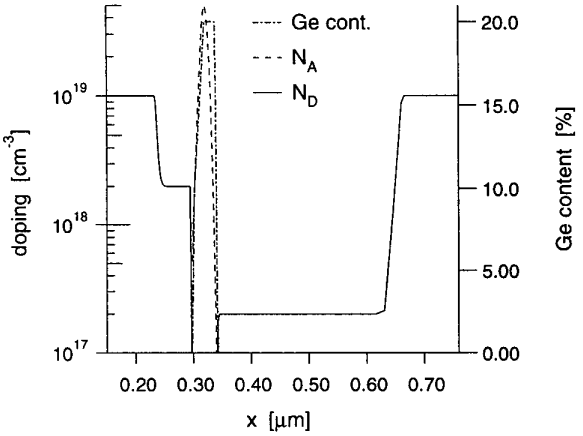


Fig. 1. Doping profile and Ge content of the HBT.

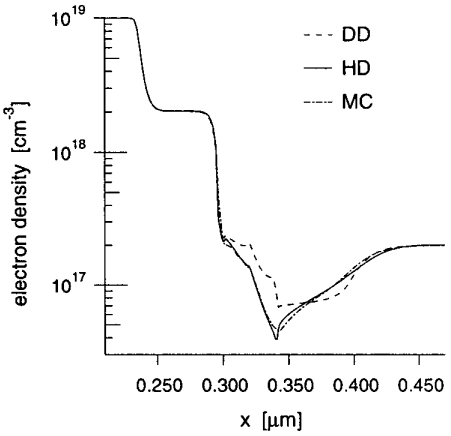


Fig. 2. Electron density for $I_C = 1.09\text{mA}/\mu\text{m}^2$ and $U_{CE} = 0.8\text{V}$.

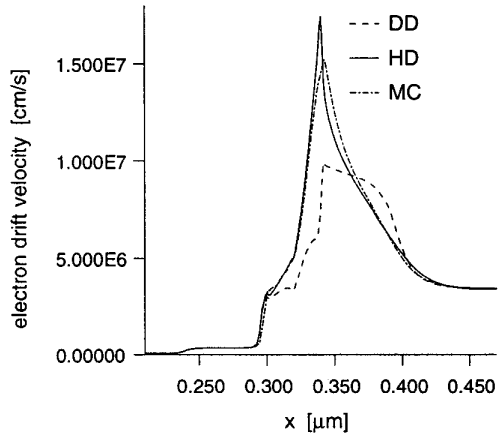


Fig. 3. Drift velocity for $I_C = 1.09\text{mA}/\mu\text{m}^2$ and $U_{CE} = 0.8\text{V}$.

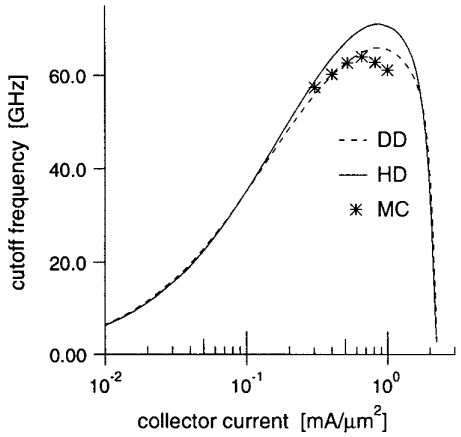


Fig. 4. Cutoff frequency for $U_{CE} = 0.8\text{V}$.

manifested in a strong velocity overshoot. While good agreement is found between the MC and HD results, the DD model fails within the base and lowly doped collector, where the transport is strongly nonohmic. At the end of the base the MC velocity is twice as large as the DD one.

The cutoff frequency is shown in Fig. 4. For small collector currents all three models yield the same cutoff frequency. This is not the case around the peak value of the cutoff frequency. The DD and HD model peak at about the same collector current, whereas the MC model has its peak at a smaller current. Furthermore, the HD model yields the highest cutoff frequency. It was expected, that the DD model yields a lower peak value, because it fails to reproduce the velocity overshoot. But it was not expected, that the MC model yields a value which is even below the DD peak frequency.

In order to find the reason for this unexpected behavior of the cutoff frequency, the transit time is evaluated for the emitter ($x < 0.298\text{nm}$), base ($0.298\text{nm} \leq x \leq 0.340\text{nm}$), and collector ($x > 0.340\text{nm}$) (Fig. 5). In the case of the collector transit time good agreement is found for all three models. Similar good agreement is obtained between the HD and MC model for the base transit time. Since the velocity in the base has only a weak dependence on the collector current, the base transit time is more or less given by the integral of the inverse velocity over the base. Since the DD model yields a velocity which is smaller than the one of the other two models, the base transit time of the DD model is the largest one. In the case of the emitter transit time the astonishing result is found, that the DD model yields the smallest transit time and the MC model the largest. The behavior of the HD model can be explained by the temperature of the electron gas which is slightly below the lattice temperature in the lowly doped emitter, because both junctions, emitter/lowly-doped-emitter and lowly-doped-emitter/base, are biased in forward direction. The barriers in these junctions lead to a stronger blocking of the cooler electron gas increasing the emitter transit time. This effect is shown in more detail in Fig. 6, where the quantity $qdn/dI_C$ is plotted for a collector current of $1.0\text{mA}/\mu\text{m}^2$. At both junc-

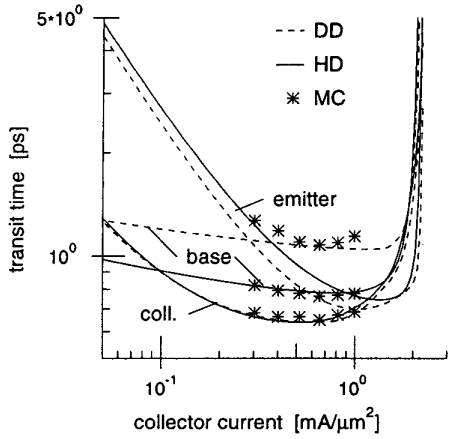


Fig. 5. Emitter, base, and collector transit time for $U_{CE} = 0.8$V.

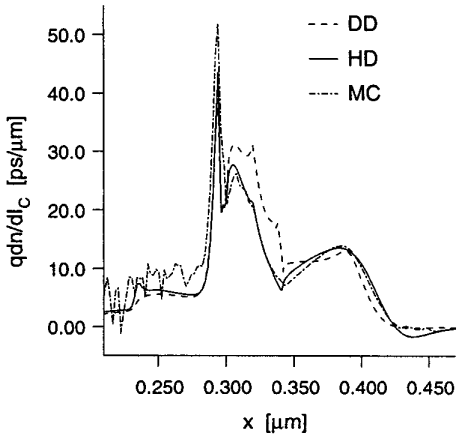


Fig. 6. $qdn/dI_C$ for $I_C = 1.0\text{mA}/\mu\text{m}^2$ and $U_{CE} = 0.8$V.

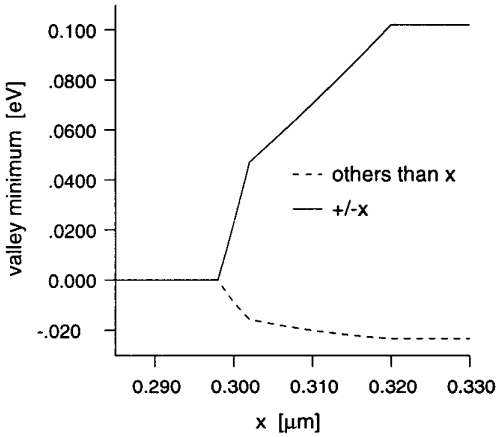


Fig. 7. Minimum energy of the different valleys of the first conduction band relative to unstrained silicon.

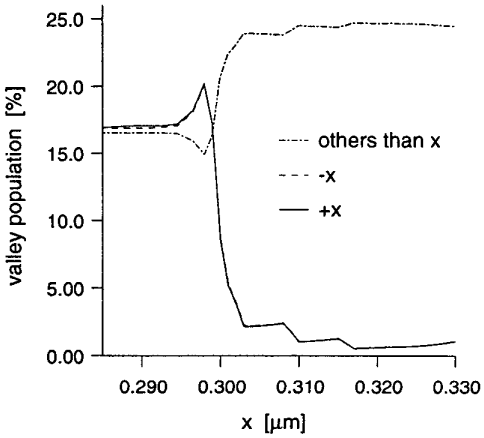


Fig. 8. Population of the valleys of the first conduction band for $I_C = 1.09\text{mA}/\mu\text{m}^2$ and $U_{CE} = 0.8$V.

tions the HD and MC results exceed the DD results. But this does not explain the much larger emitter transit time in the case of the MC model.

Although the FB-MC results in Fig. 6 are somewhat noisy in the emitter region, it can be shown that the emitter transit time discrepancy is at least partly due to the removal of the energetic degeneracy of the six valleys of the first conduction band caused by the strain in the base. The two valleys on the principal axis in $k$-space parallel to the $x$-direction are shifted upwards in energy relative to unstrained silicon, while the other four valleys are lowered (Fig. 7). Thus, particles being in the $x$-valleys encounter an increased energy barrier upon entering the base by which they might be scattered back into the emitter, whereas the particles in the other valleys encounter a lowered barrier. This behavior is reflected in the occupation of the different valleys of the first conduction band shown in Fig. 8. In the emitter region the six valleys are energetically equivalent and the populations of the six valleys are more or less equal. Close to the emitter/base junction ($x = 0.298\mu$m) the population of the two $x$-valleys is increased due to reflection at the barrier. Within the base the population of the $x$-valleys rapidly vanishes because of their energetically higher position in the $k$-space.

In the case of the DD and HD model the position-dependent band structure results in an additional force compared to the case of a uniform band structure [13]. Under the assumption that the band structure is proportional to a position-dependent factor, which is independent of the wave vector (e.g. a position-dependent effective mass), the force is proportional to the gradient of the effective density of states of the conduction band. Since only four valleys are populated in the strained base, the effective density of states is reduced to two thirds of the unstrained case. The corresponding force results in an increase of the emitter/base barrier and simulations without this force result in a strong decrease of the emitter transit time. The problem of this model is that it is based on the assumption that the

band structure is proportional to a position-dependent factor which is independent of the wave vector. This is obviously not the case in strained SiGe. Two valleys are shifted upwards in energy and four are lowered. Therefore, the factor clearly depends on the wave vector. This band structure effect is captured in full detail only by the MC model and might be the reason for the higher emitter transit time of the MC model.

Although we were not able to find other reasons for the higher emitter transit time of the MC model than the anisotropy of the band structure, our results do not unambiguously prove that the anisotropy is the only reason. In order to clarify this uncertainty further work is necessary.

## CONCLUSIONS

To our best knowledge we have presented the first transit time calculations for a bipolar transistor by FB-MC simulations. Comparison with the less CPU intensive DD and HD model reveals good agreement of the HD and FB-MC model in the collector and base region, whereas the DD model fails. In the emitter region the DD and HD model deviate from the FB-MC model, which might be due to the strong anisotropy of the strained band structure in the base of the SiGe HBT correctly described only by the FB-MC model. Further work is necessary to clarify the exact impact of the anisotropic emitter/base junction on the emitter transit time.

## ACKNOWLEDGMENT

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