On the Optimization of SiGe-Base Bipolar Transistors

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Abstract-Advanced epitaxial growth of strained SiGe into a Si substrate enhances the freedom for designing high speed bipolar transistors. Devices can be designed by altering the Ge percentage, a procedure known as bandgap engineering. An optimization study on NPN SiGe-base bipolar transistors has been performed using computer simulations focussing on the effect of the Ge profile on the electrical characteristics. In this study it is shown that the base Gummel number is of major importance on the maximum cutoff frequency and the Ge-grading itself, which induces a quasielectric field, is of minor importance. Because of the outdiffusion of the boron dope in the base and the relatively thin critical layer thickness of approximately 600 Å it appears that a box-like Ge profile with the leading edge approximately in the middle of the base is optimal. The predicted maximum cutoff frequency is 45 GHz, a sheet resistance of 8.5 k Ω/\Box and current gain of 80. The optimized device was fabricated and measurements were performed showing good agreement with the simulations.

I. INTRODUCTION

THE introduction of SiGe into conventional Si technology leads to many technical advantages. High cutoff frequencies and high current gains can be achieved using Si/SiGe/Si heterojunction bipolar transistors (SiGe HBT's) rather than Si bipolar junction transistors (BJT's), and higher Early voltages and lower sheet resistances can also be achieved.

Therefore, much research has been done on SiGe HBT's in the last years [1]–[3]. Different research groups have their own approach to forming the Ge profile. One group [2], for instance, focusses on SiGe HBT's with a uniform Ge profile in the base, while another group [3] uses graded Ge profiles.

However, both strategies are very sensitive to enhanced boron outdiffusion during a thermal anneal later on in the processing. This paper shows that a block-shaped Ge profile extending from the middle of the base region toward the collector space charge layer, offers a good compromise. The transition regions are abrupt. The optimal Ge profile was found from calculations especially of the maximum cutoff frequency $f_{t,\max}$ and the current gain H_{fe} for different Ge profiles.

A. Pruijmboom, W. B. de Boer, C. E. Timmering, and N. E. B. Cowern are with the Philips Research Laboratories, 5656 AA Eindhoven, The Netherlands. Publisher Item Identifier S 0018-9383(96)06447-7. The simulated results are compared with devices containing a graded Ge profile showing small differences in the AC characteristics. From these calculations we found that the graded Ge profile has only small influence as long as the base Gummel number is kept constant. Similar box-like Ge profiles were used in a recent publication [4] on selectively grown SiGe transistors.

Fabricating SiGe HBT's with high figures of merit can hardly be accomplished without extensive simulations. Performing simulations is necessary to optimize or predict the device characteristics. When the material parameters in the device simulators are calibrated by measurements, simulations introduce several advantages:

- Fewer processing iterations are necessary to accomplish the optimization
- Simulations give a good insight into the device physics
- The following processing "constraints" were kept in mind:
 - The device on which the simulations were applied was epitaxially grown by Atmospheric Pressure Chemical Vapor Deposition (APCVD) in an ASM Epsilon One reactor [5]. A single poly process was to be used, for which enhanced boron diffusion during the arsenic emitter outdiffusion has to be taken into account, because this would decrease $f_{t,max}$.
 - A perfectly graded Ge profile for Ge percentages beneath 5% is difficult to realize because the range of the mass-flowcontroller was such that small GeH₄ flows could not be controlled. Hence, an abrupt Ge profile is easier to grow.
 - Due to the combination of strain induced critical thickness in SiGe and boron outdiffusion, the optimizations were done for low Ge percentages (11.4% Ge). Houghton's criteria [6] was used to determine the critical thickness for this Ge percentage. Although [6] does not take into account the Si-cap layer, due to the high temperature anneal in the poly-Si processing (including a Si-cap layer) the critical thickness of 11.4 % was found to be 600 Å as was verified by our experiments.

Bearing in mind these processing "constraints," extensive one dimensional (1D) simulations were done with an inhouse device simulator (HeTRAP) with physical parameters extracted from measurements. In this simulator the unified mobility model has been implemented [7], [8]. In these simulations the cutoff frequencies were determined in the quasistatic approach.

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HeTRAP was extensively verified with MEDICI [9], a two dimensional (2D) device simulator containing the same physical models [7], [8]. For the two dimensional (2D) simulations MEDICI [9] was used for instance to examine for instance side-wall effects [10].

The task comprises optimization of an NPN SiGe HBT by calculations in order to obtain high figures-of-merit. The main concern in the transistor design based on 1D simulations appears to be the Ge profile near the emitter-base space charge region. In 2D simulations the main concern is the reduction of the product $R_b \cdot C_{\rm bc}$ and the sidewall effects for maximizing the maximum frequency of oscillation $f_{\rm max}$.

Apart from the low $R_b \cdot C_{bc}$ and high cutoff frequency f_t , the Ge profile has also to be optimized for obtaining high BV_{ce0} and ideal Gummel plots.

In Section II of this paper the models and parameters extracted from experiments and used in the simulations are described. The optimization study on a SiGe HBT is discussed in Section III by focussing on the Ge profile near the emitterbase space charge region. A comparison is made with graded Ge profiles. SIMS and DC measurements on the optimized device are discussed in Section IV. From all results a brief outline is given in Section V.

II. MATERIAL CALIBRATION

The device simulators HeTRAP and MEDICI [9] had to be calibrated with physically correct model parameters for describing the transport properties of the SiGe alloy. These parameters values are different from those in Si. The lattice constant of SiGe is larger than the lattice constant of Si. By applying a thin SiGe layer to a Si substrate, a so called strained SiGe layer arises. Consequently, the bandgap and the effective densities-of-states (DOS) in SiGe reduce compared to Si.

The bandgap narrowing (BGN) in strained SiGe is assumed to be [11]

$$\Delta E_q \approx 0.74 \cdot x \quad \text{for } x \le 0.25 \tag{1}$$

where x is the Ge percentage. In our simulations we used 11.4% Ge and thus $\Delta E_g = 84$ meV was taken. Moreover, the ratio between the product of the effective DOS

$$\frac{(N_c N_v)_{\rm SiGe}}{(N_c N_v)_{\rm Si}} \approx 0.40 \tag{2}$$

was used, as was determined from temperature dependent measurements [12], [13] by assuming Si mobility in the SiGe layer, which is correct for doping concentrations of 10^{18} cm⁻³ and higher as was shown by recent experiments for majority carriers [14]. The influence of the band-splitting on the effective DOS is a more significant factor.

Also, the unified mobility model [7], [8] was used, assuming an isotropic mobility for SiGe. The collision cross-sections depend on the effective masses, and therefore the lattice, which have been incorporated in the parameters P_i used in the model. Although not quite correct, these effective masses in SiGe are assumed to be the same in Si. Also, the mobility due to lattice scattering is considered in SiGe to be the same as in Si. Finally, the apparent BGN model [15], [16] describing the effects of heavy doping in Si was used for SiGe according to

$$\Delta E_g^{\rm app}(N) = E_1 \cdot \left\{ \ln\left(\frac{N}{N_{\rm ref}}\right) + \sqrt{\left[\ln\left(\frac{N}{N_{\rm ref}}\right)\right]^2 + C} \right\}$$
(3)

where ΔE_g^{app} is the apparent BGN, $E_1 = 6.92 \cdot 10^{-3} \text{ eV}$, $N_{\text{ref}} = 1.3 \cdot 10^{17} \text{ cm}^{-3}$ and C = 0.5 are fitting parameters and N is the doping concentration.

III. SIMULATIONS

The total transit time τ_{ec} of the bipolar transistor that determines the cutoff frequency (in quasistatic approach) is given by

$$f_t = \frac{1}{2\pi \cdot \tau_{ec}} \tag{4}$$

where τ_{ec} can be divided according to

$$\tau_{ec} = \tau_{eb} + \tau_b + \tau_c$$

and where

$$\begin{aligned} \tau_{\rm eb} &= r_e \cdot (C_{\rm eb} + C_N) \\ \tau_b &= \frac{W_b^2}{2D_n} \\ \tau_c &= \frac{W_c}{2v_{\rm eat}} + R_c \cdot C_{\rm bc} + r_e \cdot C_{\rm bc} \end{aligned}$$

where $\tau_{\rm eb}$, τ_b , τ_c are the emitter-base, the base and the collector transit times, respectively. The emitter-base transit time depends both on the compensated and uncompensated carrier charge in the E-B space charge region. The base transit time depends on stored charge in the neutral base region and the collector transit time depends on charge storage in the B-C space charge region. $C_{\rm eb}$ and $C_{\rm bc}$ are the emitter-base and base-collector depletion capacitances per unit area. W_c and W_b are respectively the B-C space charge layer thickness and neutral base thickness. C_N is the neutral or storage capacitance per unit area, caused by compensation of free carriers, R_c is the collector resistance and $v_{\rm sat}$ is the electron saturation velocity. The emitter differential resistance is given by

$$r_e = \frac{kT}{qJ_c} \tag{5}$$

where k is Boltzmann's constant, T the temperature, q the elementary charge. As mentioned in [17] the storage capacitance takes the form

$$C_N = \frac{U_l}{a} \cdot n_i \cdot e^{\frac{3}{4} \cdot \left(\frac{qV_{be}}{kT}\right)} \tag{6}$$

where a depends on the slope of the emitter profile, n_i is the intrinsic carrier concentration and U_l is the normalized potential in the E-B space charge region formulated as

$$U_l = \frac{q}{kT} \cdot \left\{ \Psi - \frac{1}{2} \cdot (\phi_n + \phi_p) \right\}$$
(7)

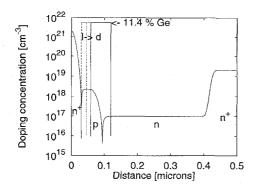


Fig. 1. The vertical doping profile of the HBT structure. The maximum Ge concentration is 11.4%. The poly-mono interface is at x = 0.

where Ψ is the potential and ϕ_n, ϕ_p are the quasi-Fermi levels of the electrons and holes, respectively.

By adjusting the vertical doping profile of a HBT structure simulations were performed and results were analyzed in order to understand the physics. Because it is not our intention to discuss the design of a traditional Si BJT vertical doping profile, we concentrate primarily on the leading edge of the Ge profile, near the emitter-base region. In Fig. 1, the vertical doping profile of the SiGe heterojunction bipolar transistor (HBT) is shown. This structure has a base doping concentration of $2.2 \cdot 10^{18}$ cm⁻³, an emitter maximum doping concentration of $2 \cdot 10^{21}$ cm⁻³ at the poly/mono interface, an epi-layer thickness of 3000 Å and doping concentration of $1 \cdot 10^{17}$ cm⁻³.

Due to the extreme high emitter doping concentration it is expected that the electrically active doping concentration is much lower, particularly at the poly/mono interface. In the simulations however, an empirically determined surface recombination velocity at the poly/mono interface of $1.4 \cdot 10^5$ cm/s was used, which also compensates for inaccuracies in the active doping concentration.

In particular the position of the leading edge of the *abrupt* Ge profile was varied over a distance d from the E-B junction (see Fig. 1). On the other hand the position of the trailing edge of the Ge profile has relatively little influence and was kept constant in the base-collector (B-C) space charge region.

In Fig. 2 $f_{t,\max}$ and the current gain H_{fe} are shown as a function of the position of the leading edge of the Ge profile relative to the E-B metallurgical junction. Three regions of operation can be seen. In region 1 the Ge edge is in the E-B space charge region. BGN increases the storage time in the E-B space charge region. Here, the Ge causes extra bandgap narrowing (BGN, see (1)) which reduces $f_{t,\max}$.

For n_i the Maxwell-Boltzmann approximation can be used according to

$$n_i^2 = N_c \cdot N_v \cdot e^{\left(\frac{-E_g}{kT}\right)} \tag{8}$$

where E_q is the bandgap.

Equation (8) clearly shows that BGN in SiGe increases n_i considerably although the effective DOS reduce and according to (6) C_N increases. Consequence is that the storage time increases resulting to a lower $f_{t,\max}$ (see Fig. 2).

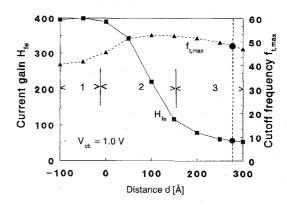


Fig. 2. The maximum cutoff frequency $f_{t,\max}$ and the current gain H_{fe} as a function of the distance d shown in Fig. 1. This so called *technical window* can be divided into three regions: 1, 2 and 3. The collector-base voltage $V_{cb} = 1$ V. The maximum values are for $f_{t,\max} = 52$ GHz and for $H_{fe} = 400$. The optimal position (x = 285 Å) is indicated with a circle (•).

Shifting the profile edge to region 2 increases $f_{t,\max}$ and decreases H_{fe} . In this region the base Gummel number is very sensitive to the bias condition V_{be} because the Ge edge is very close to the E-B space charge region. Here, the profile causes an enhancement of the base Gummel number

$$G_B = \int_0^L \left(\frac{p}{D_n}\right) \cdot \left(\frac{n_{io}^2}{n_i^2}\right) dx \tag{9}$$

where L is the device length, p the hole concentration, D_n the electron diffusion coefficient and n_{io} is the intrinsic carrier concentration in Si. This enhancement reduces the collector current density according to

$$J_{c} = -\frac{qn_{io}^{2}}{G_{B}} \cdot \left\{ e^{\left(\frac{qV_{ba}}{kT}\right)} - 1 \right\}.$$
 (10)

In region 3 the profile edge enters deeper into the neutral base region causing a considerable reduction in the collector current density J_c . Consequently, $f_{t,\max}$ reduces which is caused by the storage time that depends on G_B . By the enhancement of G_B according to (10) J_c reduces. Hence, for reaching $f_{t,\max}$ and therefore the same J_c , a higher applied V_{be} is necessary. Consequently, according to (6) a high C_N is incorporated reducing $f_{t,\max}$.

Fig. 2 gives an overview which can generally be used to optimize SiGe HBT's and is always of the same form. The slopes of both curves in the overview depend on the device structure, temperature, collector-base voltage $V_{\rm cb}$ and Ge percentage. Only region 1 and region 3 have "stable operation," i.e., ideal Gummel plots. In region 2 the Ge profile is rather close to the E-B space charge region and this causes a parasitic energy barrier that strongly varies with the applied bias V_{be} . This modulates the base Gummel number and introduces a strong nonideal I_c - V_{be} Gummel plot. If the Ge profile reaches to region 1 a much larger SiGe layer thickness would be needed increasing the risk of misfit dislocations in the material (degredation). Therefore the optimal position of the Ge profile is in region 3, that means the leading Ge edge is approximately in the middle of the base region and the trailing edge somewhere in the collector space charge layer (see Fig. 2). This is also very attractive to get a high Early

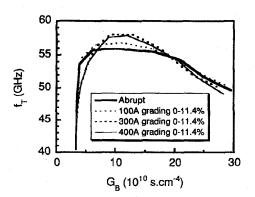


Fig. 3. The vertical doping profile used in simulations. The distance is relative to the poly/mono-Si interface (x = 0). The position of the leading edge of different Ge profiles was varied through the base. In this figure a linearly graded Ge profile is shown indicated with a slope of 11.4%/300 Å.

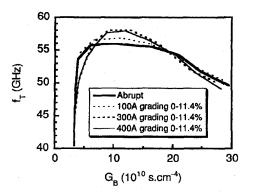


Fig. 4. The calculated maximum cutoff frequency $f_{t,\rm max}$ vs. the base Gummel number G_B (T = 300 K, $V_{\rm cb} = 0$ V). In the calculations the vertical doping profile shown in Fig. 3 has been used. The numbers 100, 300 and 400 indicate Ge profile slopes (or gradings) of 11.4%/100 Å, 11.4%/300 Å and 11.4%/400 Å Ge through the base.

voltage (V_A) as has been shown by Prinz [13]. For the Early voltage V_A it is more suitable to place the Ge profile in region 3 rather than in region 1, because the base Gummel number (see (9)) in SiGe is much smaller than in Si. Hence, most of the current is then determined by the Si layer and a change in V_{cb} causes hardly any change in the collector current when the Ge profile is applied in region 3. The current gain value in region 3 is much lower than for the Ge profile in region 1 which does increase BV_{ce0} .

At the optimal position, which is 285 Å from the E-B metallurgical junction, $f_{t,\max}$ is approximately 45 GHz, the maximum current gain $H_{fe,\max}$ is 80 and the SiGe thickness approximately 600 Å.

To make the discussion more complete, the high frequency behavior for different Ge profiles was compared: Different linearly slopes (or gradings) of the leading edge were used in the simulations (see Fig. 3). In order to increase the possible influence of the base transit time on the total f_t we reduced the collector epi-layer thickness from 3000 Å to only 1500 Å.

By analogy with earlier experiments (Fig. 1) we considered different Ge profiles with four different slopes (or gradings) (abrupt, 100 Å, 300 Å and 400 Å) with a maximum Ge

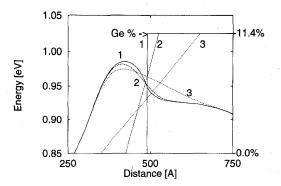


Fig. 5. A blow-up of the conduction band edge in the base region for three different Ge profiles. These profiles are indicated with "1" for the abrupt Ge profile, "2" for 100 Å, grading and "3" for 300 Å grading and are shown in the figure.

percentage of 11.4% and shifted each of the Ge profiles through the base (see Fig. 3). For every position of each profile the values for G_B and $f_{t,\max}$ were calculated (see Fig. 4). Fig. 4 shows that differences between $f_{t,\max}$ values are quite small (approximately 3.5%) confirming that $f_{t,\max}$ is mainly determined by G_B and the slope of the Ge profile has hardly any effect on the high frequency behavior. Moreover, in this plot one can see two physical effects which were discussed earlier. First, the relatively weak fall-off of $f_{t,\max}$ at higher G_B values, which can be explained with (1), (4), (8), (9) and (10) and second, a strong fall-off for G_B lower than $3.0 \cdot 10^{10}$ s.cm⁻⁴, which is caused by Ge induced BGN in the emitter-base space charge region ((1), (4), (6) and (8)).

In Fig. 5 a blow-up of the conduction band in the base is given for three Ge profiles, while the base Gummel number is kept constant $(9.5 \cdot 10^{10} \text{ s.cm}^{-4})$ near the top of the $f_{t,\text{max}}$ vs. G_B shown in Fig. 4. This figure shows the influence of the slope of the Ge profile on the decay of the conduction band. The continuity in he conduction band is due to the assumption that the electron affinity in SiGe is the same as in Si. According to People [11] nearly the total bandgap discontinuity takes place in the valence band.

In processing, it is common practice to use the base sheet resistance R_{\Box} as an optimization parameter for the high frequency behavior of Si bipolar transistors [18], which is formulated as

$$R_{\Box} = \frac{1}{q \int_0^L \mu_p p dx} \tag{11}$$

where μ_p is the hole mobility. As is well-known, the $R_{\Box} \cdot G_B$ product is approximately constant as appears in (9) and (11). However, in SiGe HBT's this product is not constant but is strongly dependent on the Ge percentage in the base. Recent experiments [14] done for boron concentrations of 10^{18} cm⁻³ and higher have shown that, for equal doping concentrations, the base sheet resistances are the same for different Ge percentages. In Fig. 4 R_{\Box} is constant and the $f_{t,\max}$ varies with the G_B . This demonstrates that the base Gummel number is essential for the optimizations of the SiGe HBT's. IEEE TRANSACTIONS ON ELECTRON DEVICES, VOL. 43, NO. 9, SEPTEMBER 1996

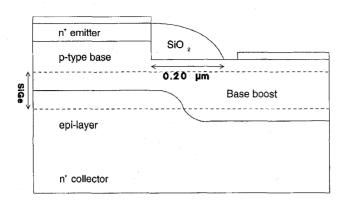


Fig. 6. A schematic cross section of the optimized 2D device structure used in all simulations. The oxide spacer and the base boost are shown in the figure.

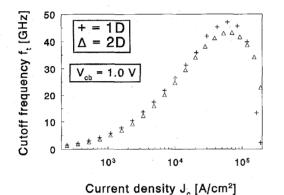


Fig. 7. Cutoff frequencies as a function of the collector current density J_c calculated with 1D (+) and 2D (Δ) simulations.

The abrupt Ge profile was chosen for the optimizations because of the strong processing "constraints". For the optimizations 1D simulations were performed, but two dimensional (2D) simulations were done to examine specific problems, such as sidewall effects and the total base resistance. These simulations are important for extracting parameters used for downscaling of transistor structures.

It was shown that sidewall effects in SiGe HBT's are reduced due to bandgap narrowing in SiGe [10]. An effective way to remove sidewall effects completely is to apply an oxide spacer (see Fig. 6). Also, the base boost was self-aligned with the oxide spacer and was optimized such that it did not penetrate deeply into the epi-layer, thus minimizing the parasitic collector-base depletion capacitance. The base boost has a maximum doping concentration of $1.5 \cdot 10^{20}$ cm⁻³. Moreover, an effective surface recombination velocity of $4 \cdot 10^4$ cm/s was used for the titan-silicide base contact and for the emitter poly/mono interface an effective surface recombination velocity of $1.4 \cdot 10^4$ cm/s was used (as in 1D simulations).

The simulations were performed on the 1D optimized device structure and the results—the calculated cutoff frequencies and current gains—were merely the same (see Figs. 7 and 8). It is noteworthy that in 1D simulations the quasistatic approach was used, while in the 2D simulations AC small-signal analysis was used, showing that the optimized 2D structure has a nearly 1D behavior.

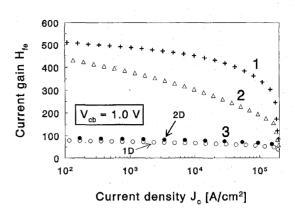


Fig. 8. The current gain H_{fe} as a function of the collector current density J_c . The numbers in the figure indicate the regions marked in Fig. 2. For region 3 both the 1D as the 2D simulations are indicated with an arrow,

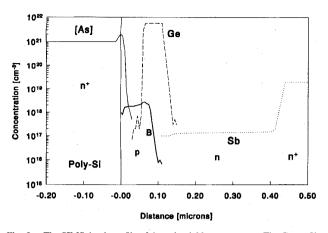
In conclusion, the 1D simulations are essential for the optimizations in general because the SiGe layer mainly affects the 1D behavior. 2D simulations are important to adjust the device to be more "1D-like" and to extract scaling effects.

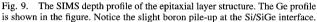
IV. MEASUREMENTS

Given the requirements and processing "constraints," especially the boron outdiffusion, the result is a HBT with a base sheet resistance of 8.5 k Ω/\Box (see Fig. 9). The transistors were grown by Atmospheric Pressure Chemical Vapor Deposition (APCVD) in an ASM Epsilon One reactor. In Fig. 9 the SIMS depth profile of the fabricated optimized device is shown. The boron pile-up at the leading edge of the Ge profile is probably due to segregation [19] caused by different solubilities in Si and strained SiGe. According to Hu [19] the same kind of pile up is not caused by an ion yield shift in the SIMS analysis of SiGe, but an actual change in the boron concentration. An important remark is that capacitancevoltage (CV) measurements have shown the same behavior in the hole concentration. This suggests a striking analogy in the theoretical descriptions concerning heterojunctions in the device and process physics. The pile up in the boron concentration appears to be electrically the same as an hole accumulation layer.

DC current-voltage measurements were performed on the 8.5 k Ω/\Box HBT (see Fig. 10). These measurements are compared with 2D simulations. The measured base current shows a stronger nonideal part for low applied $V_{\rm be}$ than in the simulations. Different measurements by altering V_{cb} have shown that it does not affect the base current, meaning that there is no recombination at the Si/SiGe hetero interface and hence that there are hardly any misfit dislocations. Moreover, 1D simulations have shown much less recombination at the emitter-base space charge region. Therefore, we conclude that the large amount of recombination is caused by the oxide spacer quality. The simulated collector current agrees well with measurements. This confirms that (1) and (2) in combination with the unified mobility model and the assumption of the apparent BGN caused by heavy doping are accurate for predicting the electrical performance of devices.

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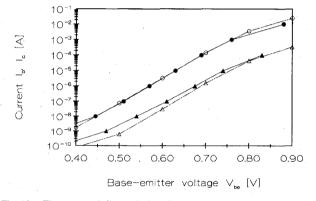


Fig. 10. The measured Gummel plot (dense marks) of the optimized HBT structure compared with MEDICI [9] (2D) simulations (open marks) for T = 294 K and $V_{\rm cb} = 0$ V.

For practical reasons the high-frequency (f_t) measurements could not be performed on the single poly SiGe HBT's, discussed in this paper. However, f_t measurements were done on double poly SiGe HBT's with the same box-like Ge profile [4] which agreed very well with the simulations.

V. CONCLUSION

This paper has shown that the base Gummel number (G_B) is of major importance for optimizations of SiGe-base bipolar transistors. It not only determines the current gain but also the maximum cutoff frequency $(f_{t,\max})$. The grading of the Ge profile is of minor importance. Incorporating a graded Ge profile for the same base Gummel number gives approximately the same results. Because of the outdiffusion of the boron dope in the base and the relatively thin critical layer thickness of approximately 600 Å it appears that a box-like Ge profile with the leading edge approximately in the middle of the base is optimal. The predicted maximum cutoff frequency is 45 GHz, a sheet resistance of 8.5 k Ω/\Box and current gain of 80. Moreover, from DC measurements it appears that the simulations predict the collector current guite correctly by considering in SiGe the Si mobility model and apparent bandgap narrowing caused by heavy doping together with the conventional formulas for bandgap narrowing and the effective densities-of-states in strained SiGe matched to a Si substrate. SIMS analysis showed a boron pile up near the Si/SiGe interface. This was probably caused by boron segregation.

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