MODELS FOR CARRIER TRANSPORT IN THE BASE OF npn SiGe HBTs

Sasa Sokolić*, Slavko Amon
Faculty of Electrical Engineering, University of Ljubljana, Slovenia
*METRONIK, Ljubljana, Slovenia

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Keywords: semiconductors, HBT, Heterojunction Bipolar Transistors, carrier transport, npn bipolar transistors, Si-Ge transistors, carrier transport modeling, minority carriers, analytical modeling, numerical modeling, BGN, BandGap Narrowing, transistor bases, diffusion constants

Abstract: Based on recalculated experimental and theoretical data, a consistent set of models for minority carrier transport in p-type SiGe HBT base is presented. Models are valid in wide range of temperature, doping level and Ge content ($77K<T<350K$, $N_A<10^{20}cm^{-3}$, $x_{Ge}<0.2$) and are appropriate for advanced analytical and numerical modeling of SiGe HBTs.

Modeli za transport nosilcev v bazi npn SiGe heterospojnega transistorja

Ključne besede: polprevodniki, HBT transistorji bipolarni heterospojni, transport nosilcev nabojev, npn transistorji bipolarni, Si-Ge transistorji, modeliranje transporta nosilcev nabojev, nosilci minoritetni, modeliranje analitično, modeliranje numerično, BGN oženje pasu prepovedanega, baze transistorjev, konstante difuzijske

Povzetek: Delo predstavlja skupek modelov za transport manjšinskih nosilcev v p-bazi SiGe heterospojnega bipolarnega transistorja, določenih na osnovi ponovno preračunanih eksperimentalnih in teoretičnih podatkov. Modeli so uporabni v širokem intervalu temperatur, dopiranja in Ge vsebnosti ($77K<T<350K$, $N_A<10^{20}cm^{-3}$, $x_{Ge}<0.2$) ter so primerni za analitično in numerično modeliranje SiGe heterospojnih bipolarnih transistorjev.

1. INTRODUCTION

Improved performance of SiGe HBTs compared to Si BJTs is closely related to the effects in the SiGe base /1/. As a consequence of germanium and related compressive strain, several phenomena appear in the base, affecting carrier transport. The most important effect - bandgap narrowing (bgn) due to strain and alloying - results in an increased electron injection from the emitter to the base and, consequently, in an increased collector current. Graded germanium profile in the base introduces graded bandgap and, consequently, an accelerating built-in electric field in the base that improves high frequency characteristics of SiGe HBTs. Beside bandgap reduction, several other effects in the SiGe base (mobility enhancement etc.) influence the device characteristics /2-9/.

Due to considerable scattering of experimental and theoretical data on SiGe materials and devices found in the literature, making their direct application almost imposible, a rigorous analysis of data available is made. It is found that different authors use in their evaluations different values for constants and material parameters, different definitions for effects involved and different formulations of models (such as $D_{n,SiGe}$, $\mu_{n,SiGe}$, n_i^2, ΔG_{SiGe} etc.). All this caused large discrepancies of reported results, in spite of excelent experimental or theoretical work performed by several authors. Therefore, all experimental and theoretical data used in our work were recalculated with the unified definitions for involved constants, parameters and models. As will be seen in the following, close agreement between recalculated data from different authors was obtained, enabling use of those data for the derivation of improved model. Models derived are adequate in a wide range of temperature T, doping level N_A and Ge content x_{Ge} ($77K < T < 350K$, $N_A < 10^{20}$ cm^{-3}, $x_{Ge} < 0.2$).

2. SiGe HBT BASE OPERATION

To get a clear insight into the transistor base operation, classical Moll-Ross /10/ approach for the calculation of base minority current j_n and transit time τ_B was applied. Assumptions of this approach are:

- Ideal homogenous base (N_A = const, n_i^2 = const, D_n = const, etc.)
- Carrier transport correctly described by Drift-Diffusion model
- Recombinations in the base neglected (R_{Base}= 0 or j_{nBase} = const)
- Low Level Injection

Moll-Ross approach was generalised for the case of nonuniform doping and band gap grading by H. Kroemer /11/

$$j_n = \frac{q(\exp(qV_{BE})-1)}{\int_0^{Wb} \frac{N_A(x)dx}{(pn)_{SiGe} D_{n,SiGe}(x)}} \quad (1)$$

$$\tau_B = \int_0^{Wb} \left[(pn)_{SiGe}(z) \int_z^{Wb} \frac{N_A(x)dx}{(pn)_{SiGe}(x) D_{n,SiGe}(x)} \right] dz \quad (2)$$

As can be seen from (1) and (2), for adequate analytical studies of HBT base properties - similar conclusion is valid also for numerical modeling - accurate models for minority carrier diffusion constant $D_{n,SiGe}$ and $(pn)_{SiGe}$-product, in whole the range of interest ($77K < T < 350K$, $N_A < 10^{20}$ cm^{-3}, $x_{Ge} < 0.2$), must be provided! Derivation of these models is the main goal of our work and will be reviewed in the following.

3. MINORITY CARRIER DIFFUSION CONSTANT $D_{n,SiGe}$

In normal HBT operation, minority carriers are nondegenerated. Therefore classical Einstein relation is valid and minority carrier diffusion constant ($D_{n,SiGe}$) is easily calculated from minority carrier mobility ($D_{n,SiGe} = (kT/q)\ \mu_{n,SiGe}$).

Modeling of minority carrier mobility ($\mu_{n,SiGe}$) in the necessary range of temperature, doping and Ge content is based on two assumptions. First, we assume that the doping and temperature dependence of minor mobility in SiGe is equal to that in Si. This assumption is applied due to similar carrier scattering mechanisms on dopants and on phonons, both decreasing the mobility. In this case, for the determination of Si mobility, Klaassen´s unified mobility model /12/ can be used. Second, we assume that mobility enhancement in SiGe, due to strain and alloying, can be treated independently from the mobility doping and temperature dependence. In this case, for SiGe minor mobility enhancement, the model of Decoutere et al. /13/ is selected. Here, enhanced minority carrier mobility in SiGe compared to that in Si, in dependence of Ge content x_{Ge}, is described by a mobility enhancement factor $D_{Ge}(x_{Ge})$, reported in /13/ as D_{nrel}.

Therefore, model for minority electron mobility in p-type SiGe base is in our case given by the following equation, joining Klaassen´s and Decoutere´s model

$$\mu_{n,SiGe}(T,N_A,x_{Ge}) = \mu_{n,Si}(T,N_A)_{Klaassen/12/}\ D_{Ge}(x_{Ge})_{Decoutere/13/} \quad (3)$$

4. $(pn)_{SiGe}$ - PRODUCT

The $(pn)_{SiGe}$-product is a fundamental parameter for bipolar SiGe device modeling, influencing many device properties. Usually in modeling, thermal equilibrium minority carrier concentrations are calculated from pn-product for given majority carrier concentrations or doping.

Adequate model for $(pn)_{SiGe}$-product, performing well in the wide temperature, doping concentration and Ge content range which is defined by the operation of real SiGe HBTs, and at the same time being appropriate for efficient modeling, does not exist at present. Work on the derivation of $(pn)_{SiGe}$-product model, taking into account available recalculated experimental and theoretical data, is reviewed in the following.

To model $(pn)_{SiGe}$-product, it is convenient to introduce apparent bgn ΔG_{SiGe}. Throughout this work we will strictly use the following definition for apparent bgn /14/

$$(pn)_{SiGe} = n_{i,Si}^2 \exp\left(\frac{\Delta G_{SiGe}}{kT}\right) \quad (4)$$

Therefore, by definition (4), apparent bgn ΔG_{SiGe} is a measure for the deviation of the pn-product in SiGe, from its value in intrinsic silicon. For reference intrinsic carrier concentration in silicon ($n_{i,Si}$), the temperature dependent model suggested by Green /17/ was selected and will be used throughout this work.

5. APPARENT BAND GAP NARROWING ΔG_{SiGe}

An expression for apparent bgn ΔG_{SiGe}, derived by Sokolić et al. /15/, will be used throughout this work

$$\Delta G_{SiGe} = \left[\Delta E_{g,hd}\right] + \left[\Delta E_{g,Ge}\right] + \left[kT \ln\left(\frac{N_{C,SiGe}N_{V,SiGe}}{N_{C,Si,i}N_{V,Si,i}}\right)\right] + \left[kT \ln\left(\frac{N_A}{N_{V,SiGe}}\right) - kTG_{1/2}\left(\frac{N_A}{N_{V,SiGe}}\right)\right] \quad (5)$$

where N_C, N_V are effective densities of states in conduction and valence band, respectivelly, and $G_{1/2}$ is the inverse of the $F_{1/2}$ (Fermi-Dirac integral of order 1/2). As seen from eq. (5), apparent bgn ΔG_{SiGe} consists of four contributions:

1. Term $\Delta E_{g,hd}$ gives bgn due to high doping
2. Term $\Delta E_{g,Ge}$ gives bgn due to Ge induced strain and alloying
3. Term with $N_C N_V$ ratio gives bgn due to lower density of states in SiGe compared to that in intrinsic Si
4. Term with ln-$G_{1/2}$ difference gives bgn due to Fermi-Dirac statistics (degeneracy)

Eq. (5) leads to an important conclusion: for apparent bgn ΔG_{SiGe} and consequently $(pn)_{SiGe}$ determination, several phenomena ($\Delta E_{g,hd}$, $\Delta E_{g,Ge}$, $N_{C,SiGe}$, $N_{V,SiGe}$) as a function of doping, temperature and Ge content must be known! The determination of those models, based on available experimental and theoretical data, remains the main goal of this work.

5.1. Effective Density of States in Conduction Band $N_{C,SiGe}$

Due to Ge induced strain and alloying, conduction band in SiGe splits into 4-fold and 2-fold degenerated bands /9/:

$$N_{C,SiGe} = 2/3\ N_{C,Si} \qquad (6)$$

For low values of x_{Ge}, also upper 2-fold degenerated conduction band states contribute to electron concentration. The model proposed by Pejćinović et al. /16/ takes this smooth transition from Si to SiGe into account. As mentioned above, we assume that $N_{C,Si}$ is described as proposed by Green /17/.

5.2. Effective Density of States in Valence Band $N_{V,SiGe}$ and hole effective mass m_p^* (N_A,T,x_{Ge})

Effective density of states in valence band $N_{V,SiGe}$ can be determined from properly defined hole effective mass m_p^* /19/, taking into account the entire effect of nonparabolicity

$$N_{V,SiGe} = 2\ (\ 2\pi\ m_p^*\ kT\ /\ h^2\ )^{3/2} \qquad (7)$$

Nevertheless, the problem of $N_{V,SiGe}$ determination remains unsolved because a closed form model for hole effective mass $m_p^*(N_A,T,x_{Ge})$ in the necessary range of temperature, doping and Ge content, and at the same time appropriate for device modeling, is not available. Existing sophisticated theoretical models are computer time consuming and difficult to be tuned with measurements – especially with transport data. Therefore, the derivation of appropriate model for hole effective mass $m_p^*(N_A,T,x_{Ge})$ is one of the major tasks in this work.

After recalculation of experimental and theoretical data found in the literature, and a critical study of different approaches to the effective mass derivation /18, 20/, a procedure for fast hole effective mass $m_p^*(N_A,T,x_{Ge})$ evaluation was proposed by Sokolić et al /25/. The procedure consists of the following steps:

1. Determination of hole effective mass for nondegenerated case $m_p^{*0}(T,x_{Ge})$
2. Determination of degeneracy transition temperature T_{deg}
3. Determination of doping dependent hole effective mass $m_p^*(N_A,x_{Ge})$ at specific low temperature
4. Construction of model for hole effective mass $m_p^*(N_A,T,x_{Ge})$. Graphic results of this model are presented in diagrams in Figs.1,2.

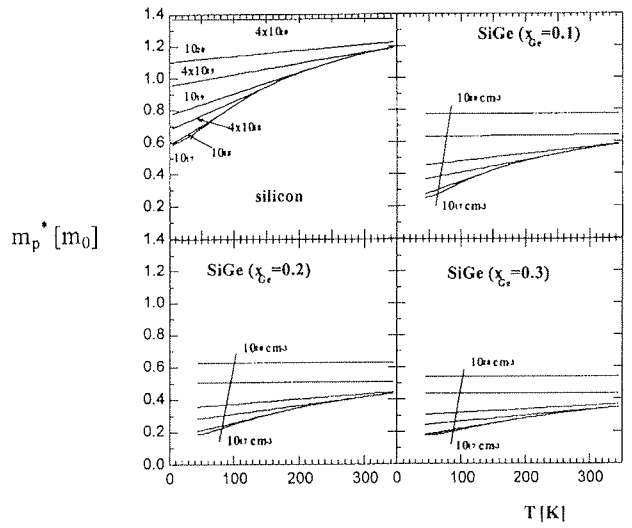

Fig.1. Calculated hole effective mass $m_p^*(N_A,T,x_{Ge})$ vs. temperature T

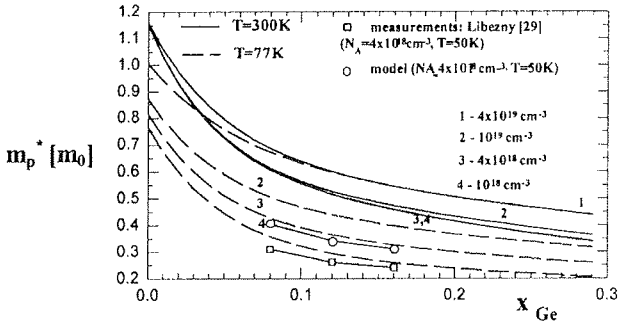

Fig. 2. Calculated hole effective mass $m_p^*(N_A,T,x_{Ge})$ vs. Ge content x_{Ge}. Experimental values for m_p^* from Libezny /29/ are shown as well.

5.3. Bandgap narrowing due to high doping $\Delta E_{g,hd}$

To determine bgn due to high doping $\Delta E_{g,hd}$, we follow a procedure proposed by Sokolić et al. /14/. The procedure is based on the following assumptions:

- in Si, we assume that $\Delta E_{g,hd}$ has a negligible temperature dependence and is only doping dependent. This assumption is generally accepted in the literature and is confirmed by both theoretical calculations of Thuselt /30/ and Jain /31/ and by experiments of Wagner /32/.
- in SiGe, we assume that $\Delta E_{g,hd}$ has negligible dependence on Ge content x_{Ge}, due to the same origin of the effect. This assumption is supported by work of Poortmans et al. /22/ and Souifi et al. /23/. Consequence of this assumption is that $\Delta E_{g,hd}$ in SiGe and in Si are equal!

Determination of bgn due to high doping $\Delta E_{g,hd}$ is based on recalculated experimental data for apparent bgn in p-type Si, obtained from measurements of I_C characteristics in Si BJTs. To enable the inclusion of the results from different authors, all experimental data had to be recalculated for the same mobility model, taken from Klaassen /12/, and for the same intrinsic Si concentration model $n_{i,Si}(T)$, taken from Green /17/. In particular, using the same procedure as proposed in Klaassen /33/, we recalculated the data for p-type Si

from Klaassen /33/ (including data from several authors) for $n_{i,Si}$ at 300K (1.08 10^{10} cm^{-3}) and the temperature dependence of intrinsic N_CN_V product ($CT^{3.43}$). In addition to $CT^{3.43}$ recalculation, the data from Poortmans et al /22/ were recalculated also for the mobility from Klaassen /12/. $\Delta E_{g,hd}$ was then evaluated from those recalculated ΔG_{Si} data by means of eq. (5), noting that in silicon $\Delta E_{g,Ge} = 0$, and that other terms can be calculated with models described above.

The final result of this procedure, bgn due to high doping ($\Delta E_{g,hd}$) vs. doping, is shown in Fig.3. It can be observed in Fig.3 that after recalculation, the experimental values from different authors are in agreement. For the purpose of analytical and numerical modeling, best fit approximation (solid line in Fig.3) was determined /14/

$$\Delta E_{g,hd} = ((a\, N_A^c)^{-4} + (b\, N_A^d)^{-4})^{-4} \quad [eV] \qquad (8)$$

where $a = 6.76\times10^{-11}$, $b = 3.58\times10^{-7}$, $c = 0.5$, $d = 0.28$ and N_A [cm^{-3}]

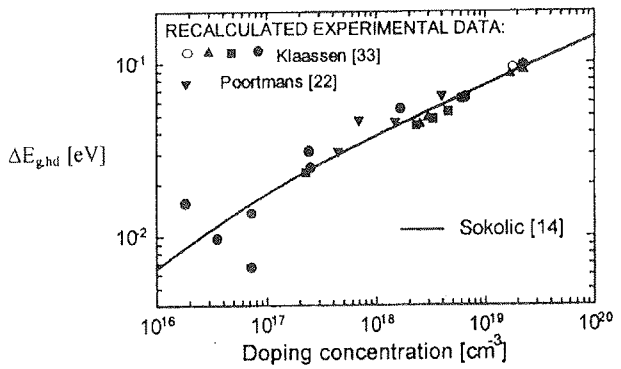

Fig. 3. Bgn due to high doping $\Delta E_{g,hd}$ vs. doping

5.4. Bandgap narrowing due to Ge induced strain and alloying $\Delta E_{g,Ge}$

To determine bgn due to Ge strain and alloying $\Delta E_{g,Ge}$, we follow a procedure proposed by Sokolić et al. /14/. Determination of $\Delta E_{g,Ge}$ is based on recalculated experimental data for apparent bgn in SiGe (ΔG_{SiGe}) and various measured effective bandgap narrowing data, obtained from measurements of I_C characteristics in SiGe BJTs. To enable inclusion and the analysis of the experimental results from different authors, all the data involved had to be recalculated for the same mobility model, taken from Klaassen /12/, for the same Ge dependence of mobility, taken from Decoutere /13/, for the same temperature dependence of N_CN_V - for intrinsic Si taken from Green /17/ and in doped Si and SiGe based on the derivations above -, for E_g in intrinsic Si as suggested by Green /17/ and for the definition of apparent bgn ΔG_{SiGe} adopted in this work, eq. (5). As a final result, bgn due to Ge induced strain and alloying $\Delta E_{g,Ge}$ is evaluated from recalculated experimental data for apparent bgn ΔG_{SiGe}, for different values of T, N_A, x_{Ge} by means of eq. (5). Note that in eq. (5), $\Delta E_{g,Ge}$ is now to be determined, ΔG_{SiGe} is measured, and other terms are calculated with models derived previously.

$\Delta E_{g,Ge}$ vs. x_{Ge} data, obtained from recalculation procedures described above, are shown in Fig.4. Recalculated data exhibit clear dependence on Ge content and almost no dependence on doping (this is not the case with row, nonrecalculated data!). It is worth mentioning that recalculated $\Delta E_{g,Ge}$ vs. x_{Ge} data points are in good agreement also with models from Bean /9/ and Robins /42/, obtained from absorbtion and photoluminescence, respectively.

All these observations lead to a conclusion that: 1. Modeling of apparent bandgap narrowing described in this work was appropriate, and 2. Recalculations of the experimental data were done correctly. In other words, we can conclude that temperature and doping dependence of effects involved were taken into account correctly with the models for m_p^* (N_A, T, x_{Ge}) and $\Delta E_{g,hd}(N_A)$ derived above.

For the purposes of analytical and numerical modeling, best fit approximation (solid curve in Fig. 4) was determined, based on recalculated $\Delta E_{g,Ge}$ values /14/

$$\Delta E_{g,Ge} = a\, x_{Ge} - b\, x_{Ge}^2 \quad [eV] \qquad (9)$$

where $a = 0.937$, $b = 0.5$ and x_{Ge} [%Ge / 100]

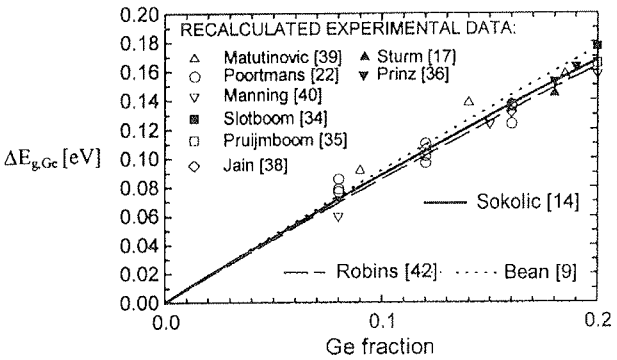

Fig. 4. Bgn due to Ge induced strain and alloying $\Delta E_{g,Ge}$ vs. Ge content x_{Ge}

5.5. Apparent bandgap narrowing ΔG_{SiGe}

With models for m_p^* (N_A, T, x_{Ge}), $\Delta E_{g,hd}(N_A)$ and $\Delta E_{g,Ge}(x_{Ge})$ derived in previous sections, apparent bgn ΔG_{SiGe} can be calculated for arbitrary N_A, T and x_{Ge} by means of eq. (5). The result of this calculation, ΔG_{SiGe} vs. doping N_A, temperature T and Ge content x_{Ge}, is shown in Fig. 5.

It can be seen in Fig. 5 that ΔG_{SiGe} increases with doping and Ge content. It can also be observed that ΔG_{SiGe} increases at low temperatures for higher Ge contents, that is due to lower influence of N_CN_V ratio at low temperatures. On the other hand, degeneracy is more pronounced at low temperatures, resulting in lower ΔG_{SiGe} at low temperatures and high doping levels. In Si, in agreement with experiments, apparent bgn ΔG_{Si} is temperature independent.

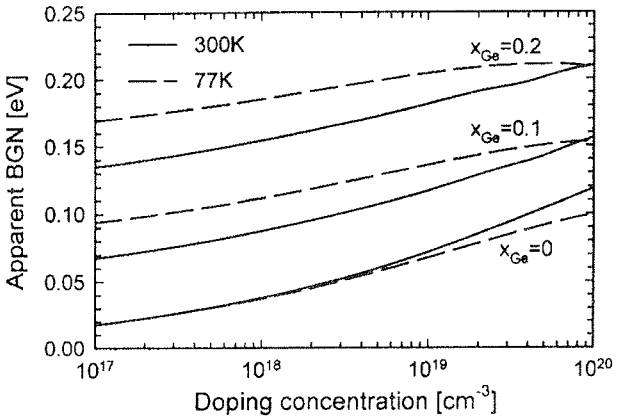

Fig. 5. Apparent bgn ΔG_{SiGe} vs. doping N_A, temperature T and Ge content x_{Ge}

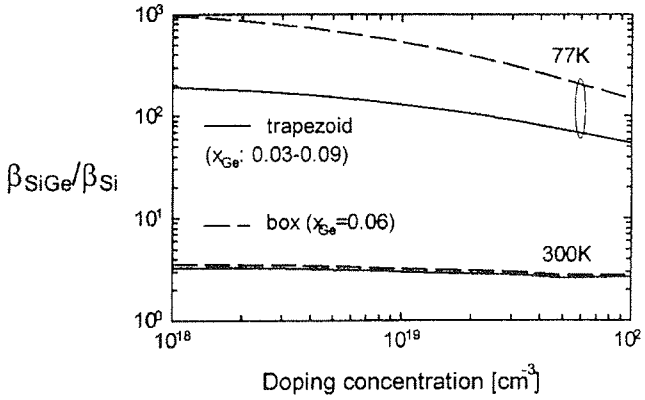

Fig. 6. Current gain ratio (β_{SiGe} / β_{Si}) vs. doping N_A

To conclude, we should not forget that all ΔG_{SiGe} curves are obtained indirectly, by considering available Si BJT and SiGe HBT measurements and can therefore, to some extent, be treated as empirical. Moreover, models for m_p^* (N_A, T, x_{Ge}), $\Delta E_{g,hd}(N_A)$, $\Delta E_{g,Ge}(x_{Ge})$ represent a consistent set of models based on available theoretical and experimental data, which determines ΔG_{SiGe} in a wide range of temperatures, doping levels and Ge content (77K<T<350K, $N_A<10^{20}$ cm^{-3}, $x_{Ge}<0.2$). It should be reminded that the entire analysis is based on $n_{i,Si}$ and $N_{C,Si}$ models suggested by Green /17/, mobility model proposed by Klaassen /12/ and Ge induced mobility enhancement according to Decoutere /13/. Finally, a Fortran or C+ subroutine based on derived models for fast calculation of hole effective mass, appropriate for numerical simulators, was concieved /28/ and is free available on Internet (http://pollux.fe.uni-lj.si/lee1).

6. APPLICATION OF DERIVED MODELS IN SiGe HBT ANALYSIS

To controll their correctness, derived models were applied in SiGe HBTs. HBT analysis is in this case based on an analytical approach (reviewed in Chapter 2). npn SiGe HBTs were studied for two Ge profiles in the SiGe base: box Ge profile /x_{Ge}=const = 6% / and trapezoid Ge profile / x_{Ge} = 3% - 9% /. SiGe HBT calculations were compared to calculations on equivalent Si bipolar junction transistor (BJT), having the same structure as HBT but no Ge. Analysis was performed at two temperatures, at room temperature (300K) and at low temperature (77K). Several basic HBT properties were studied such as current gain, base transit time, influence of Fermi-Dirac statistics etc.

6.1. Current gain

Analysis of current gain β was based on equations and models described previously in this work. Calculated current gain β for different doping and Ge profiles at 300K and 77K is shown in Fig. 6. In agreement with experimental data from the literature, it can be observed in Fig. 6 that HBT has always higher current gain β than Si BJT, due to Ge induced bandgap narrowing in the SiGe base. It can also be observed in Fig. 6 that box Ge profile results in higher β than trapezoidal Ge profile, due to higher bandgap narrowing and consequently minority carrier concentration at the base side of emitter-base depletion layer. It can be seen as well that β ratio decreases with doping. Due to the lower hole effective mass m_p^* in SiGe, Fermi-Dirac statistics becomes more influent, and apparent bgn difference (ΔG_{SiGe} - ΔG_{Si}) decreases with doping. Effect is stronger at low temperatures.

6.2. Base transit time

Analysis of base transit time τ is based on equations and models described previously in this work. Result of these calculations is shown in Fig. 7. It can be observed in Fig. 7 that, compared to equivalent Si BJT, box Ge profile results in slight decrease of transit time, due to increased minor electron mobility in SiGe. On the contrary, trapezoidal Ge profile results in a strong decrease of transit time, due to accelerating built-in electric field as a consequence of graded SiGe base. It can be observed also that transit time improvement (lowering) is smaller at high doping, due to the influence of Fermi-Dirac statistics which decreases effective Ge grading and consequently decreases accelerating electric field in the base.

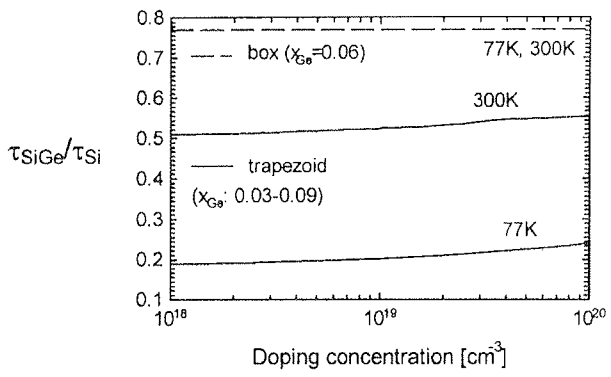

Fig. 7. Base transit time ratio (τ_{SiGe} / τ_{Si}) vs. doping N_A

6.3. Influence of Fermi-Dirac statistics

The influence of Fermi-Dirac statistics on the operation of SiGe HBT was analysed recently /24/ and recognised to be of great importance in these devices. In SiGe HBT base, greater influence of Fermi-Dirac statistics is expected than in Si BJT for several reasons - due to lower hole effective mass in SiGe, possible low temperature operation of SiGe HBT and possible high doping in SiGe base. Fermi-Dirac statistics influences minority carrier transport basicaly through two effects: major effect is Fermi level shift lowering minority electron current (4^{th} term in expression for apparent bgn ΔG_{SiGe}, eq.(5)), and minor effect is the increase of m_p^* (through 3^{rd} term in (5)), attenuating Fermi level shift.

Analysis of the influence of Fermi-Dirac statistics on SiGe HBT performance presented in this work was based on equations and models described previously in this work. Result of these calculations, minority carrier current density and base transit time ratios (Fermi-Dirac vs. Boltzmann) are shown in Fig.8. It can be seen from Fig.8 that at 300K Fermi-Dirac statistics is important for doping concentrations higher than 10^{19} cm^{-3}. At low temperatures (77K), Fermi Dirac statistics influences the device properties significantly and should be taken into account as soon as doping concentration in the base extends 10^{18} cm^{-3}. It can be concluded that due to the high doping in SiGe HBT base, Fermi-Dirac statistics should be applied for the majority of cases.On the contrary, the application of Fermi-Dirac statistics in Si BJTs - which are not well suited for low temperature operations - is important only for the highly doped emitter regions, and therefore does not affect base transport properties.

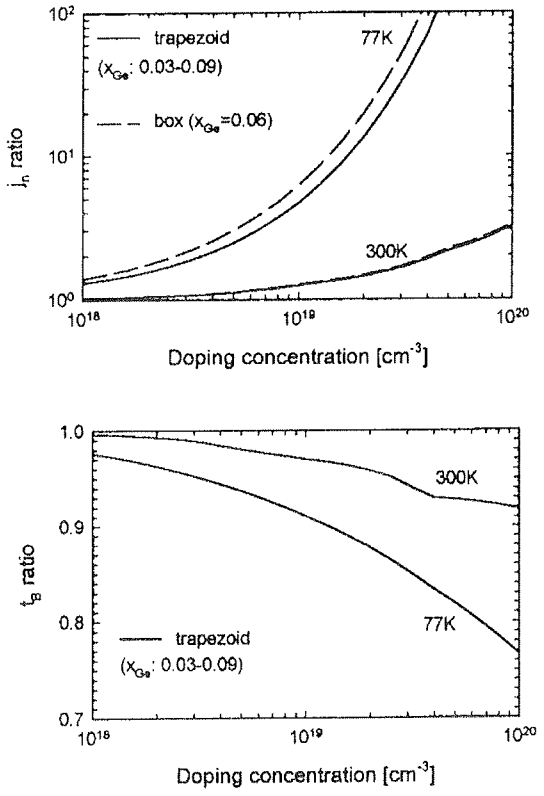

Fig. 8. Current and transit time ratio (Fermi-Dirac / Boltzmann) vs. doping N_A

CONCLUSION

A set of models for SiGe HBT carrier transport, based on criticaly and consistently recalculated experimental and theoretical data, was derived and is reviewed. Proposed set of models accounts for important effects in SiGe base such as BGN due to high doping as well as due to strain and alloying (Ge), distortion of density of states and Fermi-Dirac statistics. Proposed models are adequate for advanced analytical and numerical modeling of SiGe HBTs. A Fortran or C+ subroutine for fast calculation of hole effective mass, appropriate for numerical simulators, is free available on Internet (http://pollux.fe.uni-lj.si/lee1). Validity range of derived models is

$$77K < T < 350K\ ,\ N_A < 10^{20}\ cm^{-3}\ ,\ x_{Ge} < 0.2$$

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Sasa Sokolić, Slavko Amon*
Faculty of Electrical Engineering,
University of Ljubljana
Tržaska 25, 1000 Ljubljana, Slovenia
**METRONIK*
Stegne 21, 1000 Ljubljana, Slovenia
email: slavko.amon@fe.uni-lj.si

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