# THE EFFECT OF DOPANT OUTDIFFUSION ON THE NEUTRAL BASE RECOMBINATION CURRENT IN Si/SiGe/Si HETEROJUNCTION BIPOLAR TRANSISTORS

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### **ABSTRACT**

A new analytical model for the base current of Si/SiGe/Si heterojunction bipolar transistors(HBTs) has been developed. This model includes the hole injection current from the base to the emitter, and the recombination components in the space charge region(SCR) and the neutral base. Distinctly different from other models, this model includes the following effects on each base current component by using the boundary condition of the excess minority carrier concentration at SCR boundaries: the first is the effect of the parasitic potential barrier which is formed at the Si/SiGe collector-base heterojunction due to the dopant outdiffusion from the SiGe base to the adjacent Si collector, and the second is the Ge composition grading effect. The effectiveness of this model is confirmed by comparing the calculated result with the measured plot of the base current vs. the collector-base bias voltage for the ungraded HBT. The decreasing base current with the increasing the collector-base reverse bias voltage is successfully explained by this model without assuming the shortlifetime region close to the SiGe/Si collector-base junction, where a complete absence of dislocations is confirmed by transmission electron microscopy (TEM)[1]. The recombination component in the neutral base region is shown to dominate other components even for HBTs with a thin base, due to the increased carrier storage in the vicinity of the parasitic potential barrier at collector-base heterojunction.

### I. INTRODUCTION

In bipolar junction transistors(BJTs), it is well known that the recombination current in the space charge region(SCR) exhibits nonideal characteristics, while the hole injection current from the base to the emitter and the recombination current in the neutral base region exhibit an ideality factor close to unity. In heterojunction bipolar transistors(HBTs), the hole injection current from the base to the emitter is significantly suppressed due to the valence band offset. Therefore, the recombination current in the emitter side of the SCR becomes negligible compared to that in the base side of the SCR[2].

Major contributions to the nearly ideal base current are the recombination currents through the interface states at the heterointerface and the neutral base [2]. Since no interface states are assumed for the strained Si/SiGe heterointerface. the base current is dominated by the neutral base recombination current in Si/SiGe HBTs. For a Si/SiGe HBT with a graded base, the Fermi level is pinned to the valence band in the base and the base current is thus unaffected by the presence of Ge in the base [3]. However, even in a Si/SiGe HBT with a 500 Å-thick base and negligible defects at the collector-base(C-B) heterojunction, it has been observed that the nearly ideal base current is larger than that of Si-BJT and is also strongly dependent on the C-B reverse bias voltage [1]. Therefore, this indicates that recombination in the neutral base is responsible for the larger base current. Larger neutral base recombination current is likely caused by the presence of a high concentration of oxygen atoms inside the SiGe base. However, the dependence on the C-B bias voltage cannot be explained by the oxygen incorporation and may

be caused by other mechanisms.

Shafi et al. [1] modeled the decreasing behavior of the base current at low C-B reverse bias voltages by partitioning the neutral base region of width  $W_b$  into an abnormally short-lifetime region of width X close to the C-B junction and a conventionally long-lifetime region of width  $W_b$ -X throughout the rest of the base, even though a complete absence of dislocations at the C-B junction is confirmed by transmission electron microscopy(TEM). Therefore, the assumption of a rapid decrease of the minority carrier lifetime at the short-lifetime region becomes controversial.

In this paper, based on the boundary condition of the injected minority carrier concentration at the heterojunctions [4,5], the parasitic potential barrier effect, resulting from the bandgap alignment at the Si/SiGe interface [6] and dopant outdiffusion from SiGe base to Si collector [7,8], on the neutral base recombination current is analytically modeled and Ge composition grading effect is also included.

Then, the reduction of the base current with the increase of the C-B reverse bias voltage is successfully explained by this model without assuming the short-lifetime region close to C-B junction.

# II. MODELING

The energy band structure of n-p-n graded base Si/SiGe/Si HBTs is shown in Figure 1. In Figure 1,  $x_{je}$  and  $x_{jc}$  are the metallurgical interface of the emitter-base(E-B) and the C-B junctions;  $x_{ne}(x_{nc})$  and  $x_{pe}(x_{pc})$  are the boundaries of the E-B (C-B) SCRs;  $W_e$ ,  $W_b$ , and  $W_c$  are the thicknesses of emitter, base, and collector;  $\Delta E_c^{c-b}(\Delta E_c^{c-b})$  and

 $\Delta E_{a}^{cb} (\Delta E_{a}^{cb})$  are the conduction band and valence band offsets at the E-B(C-B) heterointerface generated by the energy band gap difference between the emitter (collector) and the base. Since the doping profile in the epitaxially grown layers of Si/SiGe HBTs is abrupt, constant doping is assumed in the emitter, the base, and the collector.

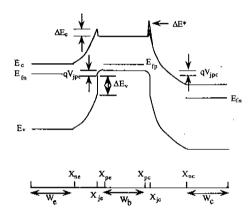


Fig. 1. Energy band structure of the Si/SiGe/Si HBTs with the ungraded base.

The excess minority carrier concentration for all injection levels has been obtained[9], using the following assumptions:

- (1) The rigid energy band model is assumed for the compositionally graded base region.
- (2) Balancing the thermionic emission flux of carriers by the diffusion flux at the SCR boundary of the heterojunction.
- (3) The flat quasi-Fermi levels of holes and electrons in the SCR.
- (4) Applying Boltzmann statistics.

(5)  $W_b$  is much less than the electron diffusion length in the base.

Based on the injection charge-based model, the electron concentration for low-level injection at the emitter and the collector edges of the base in the Si/SiGe/Si HBTs can be obtained by setting x=0 at  $x_{pe}$  and  $x=W_b$  at  $x_{pe}$  as

$$\Delta n(0) = \frac{n_{i}(0)^{2}}{N_{beff}}$$

$$\times \left[ \left\{ S'_{cn} + \exp\left(\frac{-\Delta E_{gb}}{kT}\right) \right\} S'_{en} \left\{ \exp\left(\frac{V_{bc}}{V_{T}}\right) - 1 \right\} \right]$$

$$+ S'_{cn} \left\{ \exp\left(\frac{V_{bc}}{V_{T}}\right) - 1 \right\} \right]$$

$$\div \left\{ S'_{en} S'_{cn} + S'_{cn} + S'_{en} \exp\left(\frac{-\Delta E_{gb}}{kT}\right) \right\}$$

$$\times \left[ \exp\left(\frac{-\Delta E_{gb}}{kT}\right) S'_{en} \left\{ \exp\left(\frac{V_{bc}}{V_{T}}\right) - 1 \right\} \right]$$

$$+ \left( S'_{en} + 1 \right) S'_{en} \left\{ \exp\left(\frac{V_{bc}}{V_{T}}\right) - 1 \right\} \right]$$

$$\div \left\{ S'_{en} S'_{cn} + S'_{en} + S'_{en} \exp\left(\frac{-\Delta E_{gb}}{kT}\right) \right\}$$

$$vhere$$

$$\Delta E_{gb} = E_{g}(0) - E_{g}(W_{b})$$

$$n_{i}(W_{b})^{2} = n_{i}(0)^{2} \exp\left(\Delta E_{gb} / kT\right)$$

$$S'_{en} = \frac{v_{e} \exp\left\{ \left(qV_{jnc} - \Delta E_{c}^{e-h}\right) / kT \right\}}{\left(D_{nb} / W_{b}\right) \left(\Delta E_{gb} / kT\right) \left\{ 1 - \exp\left(-\Delta E_{gb} / kT\right) \right\}}$$

$$S'_{cn} = \frac{v_{e} \exp\left\{ \left(qV_{jnc} - \Delta E_{c}^{e-b}\right) / kT \right\}}{\left(D_{nb} / W_{b}\right) \left(\Delta E_{gb} / kT\right) \left\{ 1 - \exp\left(-\Delta E_{gb} / kT\right) \right\}}$$

 $V_{be}$  and  $V_{bc}$  are the applied voltages across the E-B and C-B junctions;  $N_{beff}$  is the effective dopant concentration in the base; k is the Boltzmann constant; T is the temperature;  $n_i$  is the intrinsic carrier concentration;  $S'_{en}$  and  $S'_{cn}$  are the normalized junction velocities of electrons at E-B and C-B heterointerfaces; q is the electron charge;  $v_e$  is the mean thermal electron velocity;  $D_{nb}$  is the electron diffusion constant in the base;  $V_{jpe}$  and  $V_{jpe}$  are the potential drops across the base region of E-B and C-B SCRs. For ungraded base HBTs, equations (1) and (2) can be applied by setting  $\Delta E_{gb}$ =0. It should be noted that the base grading effect on the SCR boundaries, the potential drop across the base region of the SCR, and the built-in voltages of the junctions should also be considered as done in [10].

In Si-BJTs, the base current is composed of the hole injection current  $(I_{ep})$ , the SCR recombination current  $(I_{scr})$ , and the neutral base recombination current  $(I_{br})$ . For Si/SiGe/Si HBTs, the potential barrier for holes becomes higher by  $\Delta E_v$ , and the hole injection from the base to the emitter is thus further suppressed. Therefore, the base current is dominated by  $I_{scr}$  and  $I_{br}$  for Si/SiGe/Si HBTs. In the practical n-p-n Si/SiGe/Si HBTs, the base thickness is about 500 Å, which is much smaller than the electron diffusion length,  $L_{nb}$ . Therefore, using the equations (1) and (2), the neutral base recombination current can be approximated as:

$$I_{br} \approx \frac{qA_{e}W_{b}\left\{\Delta n(0) + \Delta n(W_{b})\right\}}{2\tau_{nb}}$$

$$= \frac{qA_{e}n_{i}(0)^{2}W_{b}}{2\tau_{nb}N_{beff}}$$

$$\times \left[\left\{1 + S_{en} + \exp(\frac{-\Delta E_{gb}}{kT})\right\}S_{en}\left\{\exp(\frac{V_{be}}{V_{T}}) - 1\right\} + \left\{\left(1 + S_{en}\right)\exp(\frac{-\Delta E_{gb}}{kT}) + 1\right\}S_{en}\left\{\exp(\frac{V_{be}}{V_{T}}) - 1\right\}\right]$$

$$\div \left\{S_{en}S_{en} + S_{en} + S_{en}\exp(\frac{-\Delta E_{gb}}{kT})\right\}$$

$$(4)$$

where  $A_e$  is the emitter area and  $\tau_{ab}$  is the electron lifetime in the base.

It has been recently reported [7] that, when the base doping concentration becomes higher than  $10^{19}$ cm<sup>3</sup>, base dopant outdiffusion from the heavily doped SiGe base into the adjacent silicon layers during the post-growth or post-annealing produces a parasitic potential barrier,  $\Delta E^*$ , in the conduction band (see Figure 1). This significantly impedes the flow of electrons to the collector [8], a pileup of electrons in the base reduces the collector current, and consequently, the recombination in the neutral base increases.

In order to consider this effect on the neutral base recombination current,  $\Delta E^*$  and the thickness of the outdiffusion region  $\Delta W_b$  are simply added to  $\Delta E_c^{\text{cb}}$  in  $S_{cn}'$  and  $W_b$  of equations (3) and (4), respectively. As the boron outdiffusion region  $\Delta W_b$  increases,  $\Delta W_b$  and  $\Delta E^*$  increase,  $S_{cn}'$  decreases, and therefore,  $I_{br}$  increases. At a given  $\Delta W_b$  and  $\Delta E^*$ , the increase of the reverse bias C-B voltage leads to the negligible increase of  $V_{jpc}$  due to the relatively heavily doped base to the collector, and therefore, the effect of  $\Delta E^*$  is dominant for low  $V_{cb}$ . But, for large  $V_{cb}$ ,  $V_{jpc}$  becomes higher and thereby the effect becomes less significant.

It should be noted that, as  $\Delta E_{gb}$  positively increases,  $I_{br}$  decreases in the normal operation (i.e. forward biased E-B junction and reverse biased C-B junction) and also increases in the inverse operation. This means that, in the normal operation, the quasi-electric field resulting from the Ge composition grading acts as the drift field to the electrons injected from the emitter while the quasi-electric field acts as the retarding field to the electrons injected from the collector in the inverse operation. Compared to the recombination lifetime of the electrons in the base, the

Ge composition grading reduces or enhances the electron transit time significantly in the normal or inverse operation, respectively. As a consequence,  $I_{br}$  decreases or increases.

By applying the boundary values of electron concentration in equations (1) and (2) to the formula of  $I_{ep}$  and  $I_{scr}$  derived in [2],  $I_{ep}$  and  $I_{scr}$ are calculated, and therefore, the base current is calculated as a sum of  $I_{en}$ ,  $I_{scr.}$  and  $I_{br.}$ 

# III. RESULTS AND DISCUSSIONS

For the different Ge mole fractions in SiGe layer, we have obtained energy bandgap [11], effective masses of electron and hole [12], and conduction band and valence band densities of states [13]. In addition to phonon, impurity, and alloy scattering mechanisms, strain is expected to play a major role in determining carrier mobility, and therefore, mobilities are different for carriers travelling parallel and perpendicular to the direction of growth. For most vertical structured HBT geometry, mobilities parallel to the growth direction are used.

Correction of these mobilities are made by replacing the effective mass in silicon with that in SiGe, and alloy scattering mobility [14] is combined with phonon and impurity scattering mobilities in silicon for majority and minority carriers (15,16) using Matthissen's rule to give the mobilities of electrons and holes in p-type SiGe base. The electron diffusion constant in the p-type SiGe base,  $D_{nb}$ , is calculated from the mobility value by using Einstein's relation or directly from the measured data by King et al. [17]. Due to the lack of data, the electron lifetime( $\tau_{nb}$ ) in p-type SiGe is assumed to be equal to that in p-type Si and obtained from the

measured data for the minority carrier in silicon [16]. The electron diffusion length  $(L_{nb})$  in p-type SiGe is calculated by the relation,  $L_{nb} = (D_{nb} * \tau_{nb})^{0.5}$ , and therefore  $L_{nb}$  is equal to 0.5 $\mu$ m for  $D_{nb}=2$ cm<sup>2</sup>/s and  $\tau_{nb}=1.2$ ns. The diffusion constants of holes,  $D_{pe}$  and  $D_{pe}$  in the emitter and the collector, respectively, are calculated from the measured hole mobility [18] using the Einstein's relation. For the doping concentrations of  $1 \times 10^{18}$  and  $3 \times 10^{16}$ cm<sup>-3</sup> in the emitter and the collector,  $D_{pe}=7.8$ cm<sup>2</sup>/s and  $D_{pc}=12.3$ cm<sup>2</sup>/s, respectively. For as-grown base doping concentration  $N_b$  equal to  $5 \times 10^{19}$  cm<sup>-3</sup>, the value of the effective base doping concentration  $N_{beff}$  in equations (1), (2), and (3) is equal to  $9\times10^{17}$ cm<sup>3</sup>, which is comparable with  $N_{beff} = 6 \times 10^{17} \text{cm}^{-3}$  used in the simulation by Shafi et al. [1].

In Fig. 2, base currents from the proposed model for the different values of parasitic potential barrier( $\Delta E^*$ ) are compared with the measured data for the Si/Si<sub>0.85</sub>Ge<sub>0.15</sub>/Si HBT [1].

For  $\sqrt{V_{hi} + V_{ch}}$  lower than about 2.8V, a good agreement is observed for  $\Delta E = 130 \text{meV}$ . Therefore, referring the measured values of  $\Delta E$ equal to 132meV for  $\Delta W_b/W_b=0.12$  [7] and 80meV for  $\Delta W_b/W_b=0.08$  ( $\Delta W_b=25$  Å and  $W_b=300\,\text{Å}$ )[8], it can be claimed that, in the test HBT with  $W_b=214 \text{ Å} [1]$ , the C-B junction may not coincide with the Si/SiGe metallurgical junction and is displaced by about 25 Å (i.e.  $\Delta W_b/W_b$ =0.12). Rapid decrease of measured base current for  $(V_{bi}+V_{cb})^{0.5}$  larger than about 2.8V could be explained by the back-injection of holes, which are generated in the C-B SCR by impact ionization. As shown in Figure 2, we successfully modeled the behavior of the base current without assuming an abnormally low lifetime of  $3 \times 10^{-13}$  sec within X=16 Å [1].

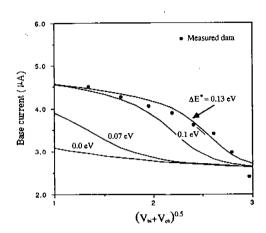


Fig. 2. Measured base current versus  $(V_{ts}+V_{cb})^{0.5}$  for the n-p-n Si/SiGe/Si HBT [1] with the Ge mole fraction of 15%. Results from the present model are also plotted with increasing parasitic potential barrier,  $\Delta E^*$ , generated by boron diffusion from SiGe base into Si collector at the C-B heterojunction. Built-in voltage  $V_{6}$  is 0.8V from device simulation. Active emitter area is  $27 \times 27 \mu$ n<sup>2</sup>.

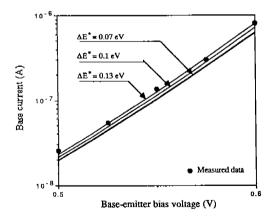


Fig. 3. Measured base current versus E-B forward bias voltage for the n-p-n Si/SiGe/Si DHBT[1] with the Ge mole fraction of 15%. Calculated base currents from the present model with increasing parasitic potential barrier at C-B heterojunction are plotted.

In Fig. 3, the effects of the parasitic potential barrier on the injected electrons from the emitter by the E-B forward bias voltage  $V_{be}$  are clearly shown. The neutral base recombination current is shown to increase with increasing  $V_{be}$ , since more electrons injected from the emitter for larger  $V_{be}$  are impeded by the parasitic potential barrier and recombined with holes.

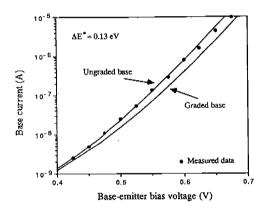


Fig.4. Base currents measured [1] and calculated by the proposed model for ungraded base n-p-n Si/SiGe/Si HBT with the Ge mole fraction of 15%. Calculated base current for Ge composition graded base HBT at ΔE\* equal to 0.13eV is also plotted for comparison. Ge composition is graded from 0 to 15% at E-B junction and C-B junction, respectively.

Fig. 4 shows the Gummel-plots of base current measured from the ungraded base HBT[1] and calculated from the proposed model for ungraded and graded base HBTs at  $\Delta E^*$  =130meV and  $V_{cb}$ =3V. In fig. 3, base current is nearly ideal for large  $V_{bc}$ , but becomes nonideal for low  $V_{bc}$ . This indicates that the neutral base recombination current becomes dominant for large bias voltages due to an increased number of injected electrons

from the emitter while the recombination current in the E-B SCR is dominant for low bias voltages. It should be noted that, as aforementioned, the recombination in the emitter region of the SCR is neglected in calculating SCR recombination current.

For the graded base HBT, there should be no discontinuity in the conduction  $(\Delta E_{\epsilon}^{\epsilon - b})$  or valence band  $(\Delta E_{\nu}^{cb})$  at E-B junction and  $\Delta E_{c}^{cb}$ of  $S_{en}'$  in equation (1) and  $\Delta E_{e}^{e,b}$  in  $I_{ep}$  [2] should be zero. Therefore, equation (1) becomes the excess minority carrier concentration of the homojunction and the carrier transport across the E-B junction is dominated by diffusion instead of thermionic emission. The effect of Ge composition grading in the base on base current is shown to be considerable for large  $V_{be}$ , i.e. base current decreases with increasing base grading. Due to the quasi-electric field in the base resulting from the base grading, the base transit time of the injected electrons from the emitter is significantly reduced compared to the electron lifetime, and therefore, the probability of recombination is lowered.

# IV. CONCLUSION

The effect of the parasitic potential barrier introduced at the C-B heterojunction by the boron outdiffusion from the SiGe base into the adjacent Si collector and the Ge composition grading effect on the neutral base recombination current have been analytically investigated by modeling those effects on the excess minority carrier concentrations at the C-B SCR boundaries. A good agreement with the measured plot of the base current versus reverse bias C-B voltage is observed. It has been shown

that the carrier pileup in the vicinity of the parasitic potential barrier results in the enhancement of the neutral base recombination current. As a result, the base current increases. Since the potential barrier is varied with the reverse bias voltage, the base current increases with the decreasing bias voltage. Therefore, due to the fact that the boron outdiffusion, generating the parasitic potential barrier, is highly probable in the thermal processes during the fabrication of the n-p-n Si/SiGe/Si HBTs, the neutral base recombination current can be significantly enhanced even for the HBTs with the ultra-thin base.

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