The Effects of Base Dopant Outdiffusion and Undoped $Si_{1-x}Ge_x$ Junction Spacer Layers in $Si/Si_{1-x}Ge_x/Si$ Heterojunction Bipolar Transistors

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Abstract—**The effects of base dopant outdiffusion and nominally undoped $Si_{1-x}Ge_x$ spacer layers at the junction interfaces of $Si/Si_{1-x}Ge_x/Si$ n-p-n heterojunction bipolar transistors (HBT's) have been studied. It has been found that small amounts of boron outdiffusion from heavily doped bases or nonabrupt interfaces cause parasitic barriers in the conduction band, which drastically reduce the collector current enhancement in the HBT's. Undoped interface spacers can remove the parasitic barriers resulting in a strongly improved collector current enhancement.**

I. Introduction

$Si/Si_{1-x}Ge_x/Si$ HBT's have demonstrated potential for high-speed bipolar transistor applications [1]. The narrow-bandgap $Si_{1-x}Ge_x$ base increases the collector current and therefore makes it possible to achieve a high emitter efficiency even with high base doping and low emitter doping. The collector current enhancement compared to an all-silicon device at a fixed base-emitter voltage V_{BE}, $I_{C,\mathrm{SiGe}}/I_{C,\mathrm{Si}}$, is a figure of merit for the HBT. In this paper it is shown that small amounts of boron outdiffusion from the heavily doped $Si_{1-x}Ge_x$ base into more lightly doped emitter and collector regions can seriously degrade the collector current enhancement by forming parasitic potential barriers for electrons in the conduction band at the $Si/Si_{1-x}Ge_x$ interfaces. To prevent the formation of these barriers, undoped $Si_{1-x}Ge_x$ spacer layers on both sides of the heavily doped base were introduced into the device structure. The devices with these spacer layers have a much greater collector current enhancement than devices without spacers.

II. Influence of Nonabrupt Junctions on Collector Current Enhancement

Consider an n-p-n HBT structure with a flat Ge profile in the base and with abrupt dopant transitions at the interfaces between the Si emitter and the $Si_{1-x}Ge_x$ base, and between the $Si_{1-x}Ge_x$ base and the Si collector. The entire base layer is heavily doped with boron in a box-like profile. For such a device, the collector current enhancement at fixed V_{BE} compared to a similar homojunction device should be [2], [3]

$$\frac{I_{C,\mathrm{SiGe}}}{I_{C,\mathrm{Si}}} = \frac{D_{n,\mathrm{SiGe}}}{D_{n,\mathrm{Si}}} \frac{(N_C N_V)_{\mathrm{SiGe}}}{(N_C N_V)_{\mathrm{Si}}} \frac{(W_B N_A)_{\mathrm{Si}}}{(W_B N_A)_{\mathrm{SiGe}}} e^{\frac{\Delta E_V}{k_B T}} \quad (1)$$

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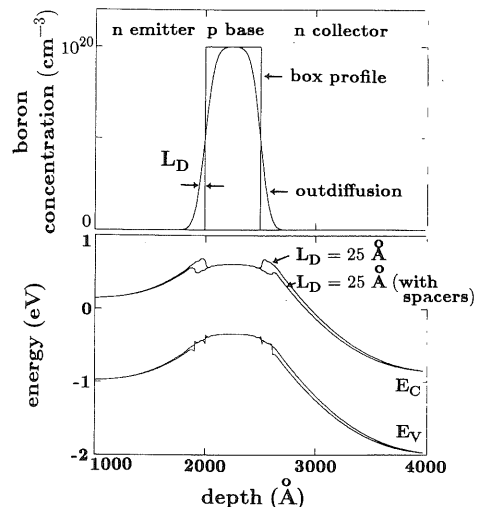

Fig. 1. Boron concentration of HBT structure used in simulating the effect of boron outdiffusion on device performance, and resulting band diagrams for $V_{BE} = 0.5$ V and $V_{BC} = -0.5$ V, with and without 100-Å-thick undoped SiGe spacer layers.

where the subscripts SiGe and Si refer to the heterojunction and homojunction device, respectively. D_n is the minority-carrier diffusion coefficient, N_C and N_V are effective densities of states in the conduction and valence band, respectively, W_B is the base width, and N_A is the base doping. The valence-band discontinuity ΔE_V for a strained $Si_{1-x}Ge_x$ layer grown on < 100 > Si is close to the total bandgap difference between Si and SiGe [4].

However, mixing and autodoping at interfaces during growth or boron outdiffusion into the adjacent silicon layers during growth or high-temperature steps in subsequent device processing can move the electrical p-n junction into the silicon emitter and collector layers. This will be shown to cause parasitic barriers for electrons at the interfaces, which will significantly degrade the collector current enhancement.

To model this effect, the HBT structure shown in Fig. 1 is considered. The base, a strained layer of $Si_{0.80}Ge_{0.20}$, is doped 10^{20} cm^{-3}, much higher than emitter and collector which are doped 10^{17} cm^{-3}. For constant diffusion coefficient D_B, dopant outdiffusion can be modeled by

$$N_A(x) = \frac{N_A^0}{2}\left(\mathrm{erf}\frac{W_B/2 - x}{2L_D} + \mathrm{erf}\frac{W_B/2 + x}{2L_D}\right)$$

where $L_D = \sqrt{D_B t}$ and N_A^0 is the doping level of the initial box profile. The one-dimensional device simulator SEDAN III

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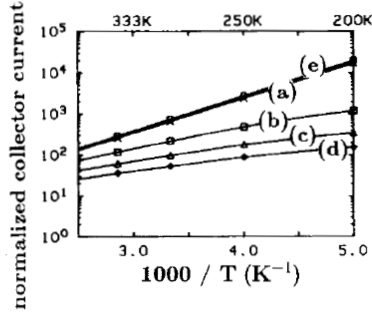

Fig. 2. Simulated normalized collector current versus inverse temperature for varying amounts of outdiffusion: (*a*) no outdiffusion (box profile), (*b*) $L_D = 25$ Å, (*c*) $L_D = 50$ Å, (*d*) $L_D = 75$ Å, and (*e*) $L_D = 25$ Å (with 100-Å spacers).

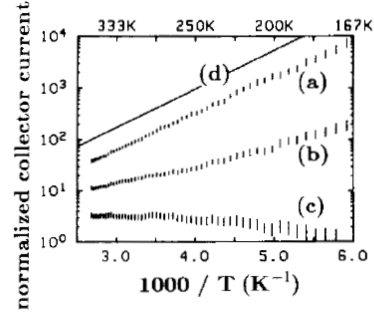

Fig. 3. Data showing normalized collector current of HBT devices with and without spacers for devices with approximately 20% Ge in the base: (*a*) $N_A = 10^{19}$ cm^{-3}, without spacers; (*b*) $N_A = 10^{20}$ cm^{-3}, with spacers; (*c*) $N_A = 10^{20}$ cm^{-3}, without spacers; and (*d*) predicted by (1) for no outdiffusion and $\Delta E_V = 150$ meV.

[5], modified for $Si/Si_{1-x}Ge_x$ heterojunctions using the values of conduction- and valence-band discontinuities from [4], was used to calculate band diagrams and collector currents for various temperatures. The band diagrams in Fig. 1 for forward-biased base–emitter and reverse-biased base–collector junctions ($V_{BE} = 0.5$ V, $V_{BC} = -0.5$V) show that even small amounts of outdiffusion cause large parasitic barriers for electrons at both heterojunctions. For example, for an outdiffusion length of 25 Å, a parasitic barrier of height 80 meV is formed at the base–emitter junction. These barriers will, of course, significantly impede the flow of electrons from emitter through base to collector, thereby degrading the collector current enhancement and thus the emitter efficiency of the device. Note that the overall barrier for holes traveling from base to emitter (one component of the base current) is unchanged. Simulated values (modified SEDAN III) of the collector current enhancement for the structures of Fig. 1 are plotted logarithmically versus inverse temperature in Fig. 2. The device with the box-like profile ($L_D = 0$ Å) has a collector current enhancement similar to that described by (1), whereas the devices with outdiffusion have a significantly degraded collector current enhancement as expected. Note that the outdiffusion reduces the slope of the collector current enhancement versus inverse temperature even more than the collector current enhancement itself. In this case (1) cannot be used to describe the collector current enhancement, and a simple "effective" ΔE_V is not a good approach to describe device performance. Once the parasitic barriers occur, the device performance is degraded and cannot be significantly recovered by further lowering the bandgap in the base. For this reason, bandgap narrowing due to heavy doping in the base was not included in this first-order model. Also shown in Figs. 1 and 2 are the band diagram and normalized collector current of a device with $L_D = 25$ Å, in which undoped $Si_{1-x}Ge_x$ spacers of thickness 100 Å have been inserted into both sides of the heavily doped base. These spacers keep the electrical junction from moving into the silicon emitter and collector and prevent the formation of parasitic barriers despite small amounts of outdiffusion. Simulation (Fig. 2) shows that with the spacers, near-ideal device performance can be recovered.

III. Device Structure and Experimental Results

Test transistor structures were grown *in situ* on < 100 > n-type silicon substrates using rapid thermal chemical vapor deposition (RTCVD) in a lamp-heated system [6]. After chemical cleaning, the wafers were loaded into the RTCVD reactor and baked in hydrogen at 1000°C for 2 min. Using dichlorosilane and phosphine in hydrogen carrier gas, heavily doped n^+ buffer layers and n-type collector layers doped $\sim 5 \times 10^{17}$ cm^{-3} were grown at 1000°C. Then p-type $Si_{0.80}Ge_{0.20}$ base layers, 300 Å thick and doped either 10^{19} cm^{-3} or 10^{20} cm^{-3}, were grown at 625°C using dichlorosilane, germane, and diborane. Finally, n-type emitter layers doped 10^{17} cm^{-3} were grown at 850°C for 3 min. Transmission electron microscopy on similar structures showed a negligible number of misfit dislocations (spacing greater than 10 μm); we conclude therefore that our base layers were strained. In some of the device structures undoped $Si_{1-x}Ge_x$ spacer layers were added on both sides of the base. The spacers, nominally 80 Å thick, were an attempt to mitigate the deleterious properties of outdiffusion and mixing as described above. HBT's were fabricated using a planar process, first used by King *et al.* [3]. Individual devices were isolated by plasma-etched mesas. Base contact was established by boron implants. To improve the emitter contact, a shallow arsenic implant was used. The devices were passivated with a SiO_2 film deposited by plasma deposition at 350°C. The implants were then annealed for 10 min at 800°C. Titanium/aluminum metallization and patterning completed the processing.

The collector current was measured as a function of base–emitter voltage at temperatures between 167 and 373 K. For current levels below the onset of high-level injection, the measured collector current was exponentially dependent on base–emitter voltage ($I_C \propto \exp(qV_{BE}/nk_BT)$), with an ideality factor n better than 1.05. In this ideal regime of base–emitter voltage, an exponential was fit to the measured collector currents. This curve was then normalized to the one of a Si homojunction device with base doping of 1.1×10^{19} cm^{-3}. As done with the simulated data in Fig. 2, the ratio of experimental collector currents, corrected for the different Gummel numbers, was plotted versus inverse temperature for zero base–collector bias in forward mode (emitter up) (Fig. 3). For all devices, the collector current enhancement was only weakly dependent on base–collector voltages between 0 V and a reverse bias of -0.5 V, and measurements in forward mode and reverse mode (emitter down) agreed well. This is expected because of the symmetrical device structure. For devices without spacers and a base doping of 10^{19} cm^{-3}, the collector current enhancement versus inverse temperature can be fitted well with (1), with a ΔE_V of 143 meV, close to that of [4], and a prefactor of about 0.3, which might be caused by different effective densities of states in the Si and SiGe layers [7]. This indicates negligible base dopant outdiffusion or barrier formation in these devices. For heavier base doping ($\sim 10^{20}$ cm^{-3}), serious degradation occurred in devices without spacers, indicating significant barrier formation from

outdiffusion or mixing. That degradation in heavily doped devices occurred indicates that the parasitic effect of the barriers is much larger than any beneficial effect of bandgap narrowing in the heavily doped bases. More severe degradation is expected for higher doped bases because of the higher doping levels in the outdiffusion tails and because of the linear dependence of the boron diffusion coefficient on boron concentration [8]. In the heavily doped case, spacers improved the device performance significantly, increasing the collector current enhancement at room temperature from 3 to 19. The performance was still not ideal, however, possibly due to inadequate spacer thickness.

IV. Conclusions

Nonabrupt base–emitter and base–collector interfaces in $Si/Si_{1-x}Ge_x/Si$ HBT's can shift the electrical junctions into the Si emitter and collector layers. The resulting parasitic barriers for electrons reduce the collector current enhancement. They can be removed using undoped $Si_{1-x}Ge_x$ spacer layers for improved device performance.

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