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Quantitative Measurement of Reduction of Boron Diffusion by Substitutional Carbon Incorporation

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Abstract

Recently, the suppression of boron diffusion due to both thermal and transient enhanced diffusion (TED) has been demonstrated through the incorporation of 0.5% substitutional carbon in the base of Si/SiGe/Si heterojunction transistor's (HBT)[1,2]. Because the devices are sensitive to diffusion on a scale less than that we can detect with SIMS, in this paper combined process and device modeling (TMA TSUPREM4 and MEDICI) are used to relate observed electrical characteristics (collector saturation currents and Early voltages) of the HBT's to boron diffusion, with a sensitivity of 20-30Å. Boron diffusivity in the SiGeC base is ~8 times slower than that of the boron diffusivity in the SiGe base without implant damage (no TED). In the case of ion implant damage in an overlying layer to cause TED the excess interstitial concentration due to ion implant damage is reduced by approximately 99% through incorporation of 0.5% substitutional carbon in the HBT SiGe bases. This demonstrates that carbon incorporation acts as an effective sink for interstitials.

Introduction

Si/SiGe/Si heterojunction bipolar transistor (HBT) technology has achieved record high frequencies for silicon compatible devices with low base sheet resistances because boron doping levels of ~$10^{20}/\text{cm}^3$ in the bases are crucial to this result [3]. However, HBT electrical performance is very sensitive to the formation of conduction band barriers at the emitter/base and base/collector interfaces due to small amounts of boron outdiffusion during processing leading to dramatic reductions in collector current and early voltages [4] (see figure 1). Recently, through the intentional introduction of high concentrations of substitutional carbon, the reduction of boron outdiffusion has been demonstrated for both annealing, and implantion and annealing conditions, greatly increasing the thermal budget for HBT targeted processes [1,2].

The reduction of boron diffusion and its transient diffusion in and near carbon-rich silicon or silicon-germanium has gathered much attention recently for its potential technological applications to control boron diffusion in processes that have ever increasingly restricted geometries [5,6,7]. In this paper we seek to quantify the reduction of boron diffusion. Because the devices are greatly affected by diffusion at levels too small to be detected by SIMS, we use modelling of the device electrical characteristics to infer the changes in boron profile and hence the changes in boron diffusion coefficients.

In n-Si/p+SiGeC/n-Si HBTs, as boron diffuses from the p+SiGeC base into n-Si emitter and collector, parasitic barriers are formed in the conduction band which impede the flow of electrons from the emitter to collector [2,8]. The parasitic barrier that arises due to boron outdiffusion is strongly dependent on the boron concentration that diffuses into the silicon, and small amounts of boron outdiffusion L_d~10Å can already cause large parasitic barriers evident in HBT's [8] because the collector current is exponentially dependent on the barrier height. This can be observed by directly measuring collector saturation current, or even more sensitively by observing the effect of collector-emitter bias on collector current (the Early effect).

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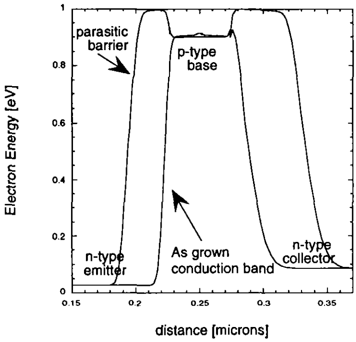

Figure 1 Qualitative conduction band diagram of a (n-)Si/(p+)SiGeC/(n-)Si HBT as grown and after annealing showing the creation of a parasitic conduction band barrier as a result of boron diffusion from the base into the n-type Si emitter and collector region.

The Early voltage changes because the barrier height, and hence the collector current, is affected by the collector-emitter bias. In this paper we use HBT electrical characteristics to quantitatively compare boron diffusion in SiGe to boron diffusion in SiGeC for annealing or implant and annealing conditions. We report that boron diffusion in SiGeC at 855°C is 1/8th that in SiGe, that the SiGeC layer acts as an interstitial sink for ~99% of the excess interstitials due to ion implant damage, and that the HBTs are far more sensitive to boron diffusion than SIMS.

Experiment

The HBT's were grown by RTCVD [9] at 575-700°C, with boron levels in the base of $\sim 10^{20}/\text{cm}^3$ and bases of ~20 nm of $Si_{0.8}Ge_{0.2}$ or $Si_{0.8}Ge_{0.2}C_{0.005}$. The device fabrication was done using all low-temperature processing to avoid unnecessary diffusion and is described elsewhere [1,2]. Photoluminescence and X-ray diffraction studies on similar alloy layers show that the alloy layers are biaxially compressively strained to match the silicon lattice, and transmission electron microscopy (TEM) showed no dislocations, defects, or SiC precipitates in any of the as-grown layers [2]. As-grown Gummel plots and common emitter characteristics of HBT's without and with 0.5% substitutional carbon in the bases are shown in figures 2(a) and (b) respectively. High Early voltages and SIMS verifies that there is no significant boron outdiffusion [1,2] in such HBT's fabricated without annealing.

Two different cases are considered for HBT processing to study boron outdiffusion. Case (1): the effect that substitutional carbon has on the intrinsic boron diffusion rates (N_2 anneal, 15 minutes, 800-950°C); and case (2): The effect of substitutional carbon on the transient enhanced diffusion of boron due to ion implant damage in the overlying emitter layer ($1.5\times10^{15}/\text{cm}^2$ 30 keV and $3\times10^{14}/\text{cm}^2$ 15 keV into the silicon 2000Å n- emitter) with subsequent 15 minute activation anneals in N_2 at 647°C and 742°C.

SIMS, Gummel plots and common emitter characteristics of the processed HBT's with ion implant damage are shown in figure 2. Saturation currents and Early voltages were then extracted from the electrical characteristics for comparison and fitting to simulated electrical characteristics. The decrease in Ic and reduced Early voltages in the transistors annealed at 647°C without carbon, figure 2 (a), show that boron has outdiffused even though this annealing condition is far less than the emitter thermal budget. However the high Early voltages in the HBT devices with carbon show that much of the TED effects have been suppresed. However, even in this case the Early voltage is not as high as that of the as grown HBTs, evidence that some slight TED effects still remain, despite no evidence of boron

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outdiffusion at 647°C in boron profiles obtained using SIMS. Figure 2 (b) shows that boron outdiffusion is readily apparent for As implantation and a 755°C, 15 min N_2 anneal in the transistor without carbon, but is substantially reduced in the transistor with carbon.

Dopant profiles were modeled using TSUPREM4 (TMA), and the results were used in the device simulator MEDICI (TMA). The diffusion coefficient (case 1) and excess interstitial concentration (case 2) were adjusted in TSUPREM so that the output of the device simulator matched the experimentally measured Gummel plots and common-emitter characteristics. In case 1 a single effective diffusion constant, D_{eff}, for boron was used to fit electrical data for the entire device structure, maintaining the ratio of neutral and singly charged defect contributions to the diffusion constant and only varying the default magnitude by a constant. In case 2 (arsenic implant) The number of excess interstitials resulting from implant damage leading to enhanced boron diffusion was scaled to match the experimentally extracted electrical characteristics, while using a typical diffusion constant of boron in silicon at 647°C of 9.33×10^{-10} um^2/min corresponding to a boron diffusion length of approximately 1Å.

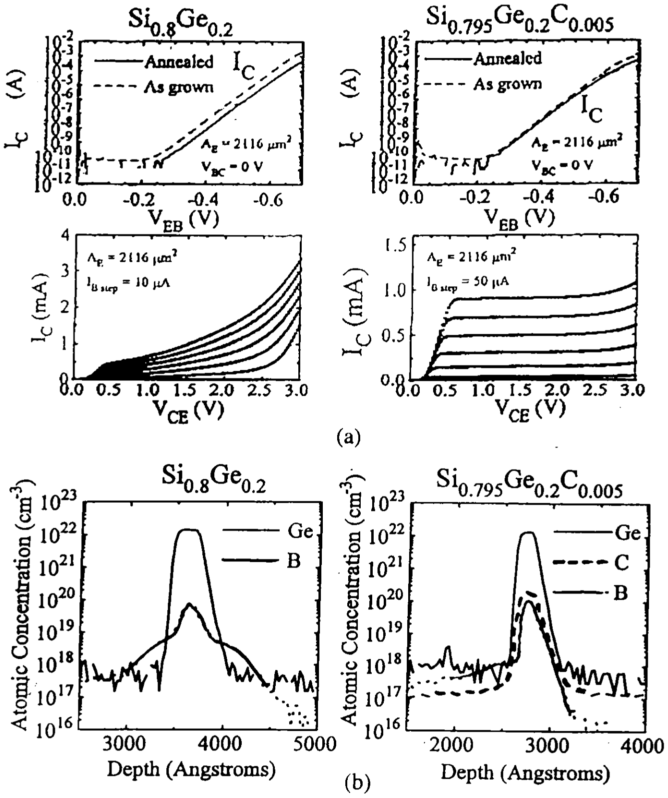

Figure 2 (a) HBT Gummel plots and collector current vs. base-collector voltage after implant into 2000 Å Si n- emitter and 647°C anneal for HBT's with SiGe or SiGeC bases. (b) boron, carbon and germanium profiles of HBT's after implant into emitter and anneal at 755°C in N2 for 15 minute [1,2]. Note: no difference in boron concentration profiles of the implanted and 647°C annealed HBTs was observed from the SIMS profiles.

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The HBT electrical characteristics were numerically simulated using the doping profiles obtained above to make comparison to experimental data. Bandgap differences of 160 meV and 147 meV were used for SiGe and SiGeC bases respectively. The effective density of states in the $Si_{1-x}Ge_x$ base, approximately $\frac{N_C N_V^{SiGe}}{N_C N_V^{Si}} \cong 0.33$ for x=0.2, is assumed not to change in the SiGeC base; and a bandgap narrowing model commensurate with observed bandgap narrowing in SiGe due to high doping densities in SiGe [10], which is less than that observed in Si, was also included.

Results & Discussion

Collector saturation currents (y axis intercept) extracted from gummel plots (collector current vs. base emitter voltage) of fabricated HBT's for case I, intrinsic diffusion, are shown in figure 3. Typical boron diffusion lengths in silicon at 855°C for 15 minutes are ~75Å [15]. The saturation current of the Si/SiGe HBT's annealed at 855°C is already reduced nearly two orders of magnitude demonstrating the extreme HBT sensitivity to small boron diffusion lengths. For HBT processing this sensitivity is undesirable because it limits the total thermal budget available to the process engineer. Through the addition of substitutional carbon the onset of saturation current degradation can be shifted to higher temperatures increasing the available thermal budget, in this case, by as much as ~100°C.

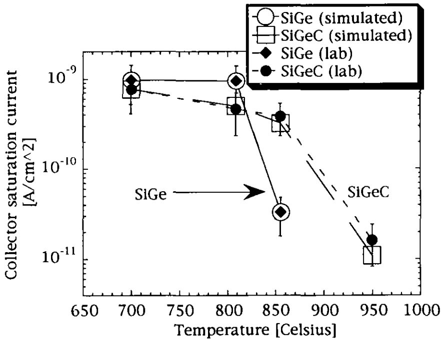

Figure 3 HBT saturation currents extracted from Gummel plots of fabricated and numerically simulated devices. Fabricated devices are indicated by solid markers, numerically simulated by hollow markers. Note carbon incorporation increases thermal budget of HBT process ~100°C.

To quantitatively estimate the relative boron diffusion constants in SiGe and SiGeC, the experimentally observed collector saturation currents were numerically calculated and fit, see figure 3, to a single diffusion parameter. The numerically obtained diffusion constants for boron in the SiGe and SiGeC are compared to that of silicon [15] in figure 4. The fitted boron diffusivities in SiGeC are uniformly slower than those in Si and SiGe. Simple best fits, using the same boron diffusion activation energy as that in silicon, yield boron diffusivities in SiGeC that are ~8 times less than that in SiGe. This agrees with previously reported boron diffusivities in SiGe and SiGeC that find boron to move slower in SiGeC than in SiGe and both diffusivities to be slower than that in silicon [12,13], but the absolute diffusivities extracted from the HBT data are approximately 2-3 times faster than those reported. Various sources of error can contribute to disagreement with the referenced values. The numerically calculated profiles are simulated with a single diffusion constant for boron. The extracted diffusivity will represent an average diffusivity of that in the alloy layer and that in silicon. For long difffusion lengths, with respect to the width of the HBT base, the numerically found boron diffusivity in the alloy should be faster than that of the actual boron diffusivities in the

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alloy. However the extracted boron diffusion lengths are small enough that relatively very little boron is found in the silicon, compared to the total boron dose in the HBT base, so this should represent only a small correction to the extracted diffusivities. Other sources of the disagreement between the reported values and ours can come from errors in temperature calibration, which can easily lead to factors of two in diffusivity; and dislocation defects which can act as interstitial sinks leading to an observed boron diffusivity slower than that in the alloy layers without dislocations. TEM studies on the as grown samples of this experiment showed no dislocations.

To illustrate the HBT sensitivity to boron diffusion, the extracted diffusion constant for boron in the 855°C annealed SiGeC device can be used to calculate an approximate boron diffusion length of ~25Å. This diffusion length is discernibly signaled by a one-half drop in collector saturation current compared to that of the as-grown HBT. However, such a small diffusion length would be nearly impossible to resolve by SIMS since broadening of the boron profile in SIMS can be of the order of 20-40Å [13], thus making HBT electrical characteristics more sensitive than SIMS to small diffusion lengths of boron.

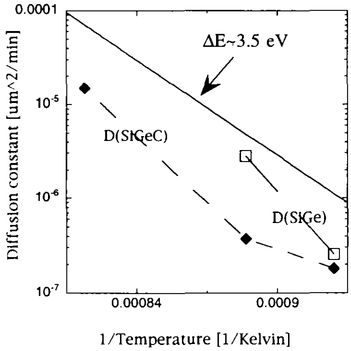

Figure 4. Boron diffusion constants obtained from fitted collector saturation currents in figure 3 . Note boron diffusivity in SiGeC ~8 times less than that in SiGe. Reference line shows activation energy of 3.5 eV.

For case 2 (ion implant damage in overlying emitter layer) Early voltages were extracted from both fabricated devices (see figure 5) and calculated using numerical simulations of the arsenic implant and anneal at 647°C. Excess interstitials due to ion implant damage lead to TED of boron and degrade device performance. The total excess interstitial concentrations were adjusted as the single parameter to fit the observed Early voltages of the devices. The unadjusted model estimates the excess interstitial concentration from implant damage to be $\sim 1.31\times10^{14}/cm^2$, and predicts a 0.3 Early voltage agreeing well with experiment. In the case of a SiGeC base, the calculated Early voltage could only be made to agree with the observed device Early voltage after a reduction of over 99% of the excess interstitials. This corresponds to a diffusion length of only a few Angstroms, again showing the sensitivity of the device to minute amounts of boron diffusion, while no difference in SIMS profiles in that case could be seen. Differing boron profiles between HBT's with and without carbon could only be distinguished by SIMS for the case of higher annealing temperature of 755°C (see figure 2).

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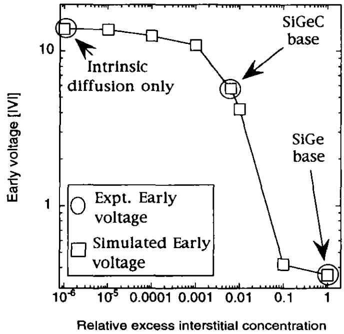

Figure 5 Calculated Early voltages for adjusted excess interstitials due to implant damage. Experimentally observed Early voltages obtained from HBT common-emitter electrical characteristics for asgrown HBTs with SiGeC bases, and implant and annealed HBTs with SiGe and SiGeC bases are indicated by circles.

Conclusions

To summarize, HBT electrical characteristics are used to determine relative boron diffusivities and excess interstitial concentrations for SiGe and SiGeC, because HBT electrical characteristics are more sensitive than SIMS to small boron diffusion lengths. The intrinsic diffusivity of boron in SiGeC is found to be approximately 8 times slower than that in SiGe, and the incorporation of substitutional carbon presents an effective sink for approximately 99% of the excess interstitials produced by ion implant damage.

Acknowledgments

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