Investigation into Inhibitory Effect of C Incorporation on Diffusion of B in SiGe

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Abstract. In this paper, the effect of C incorporation on the out-diffusion of B dopant in SiGe during high-temperature annealing and the out-diffusion of B dopant at different annealing temperatures were studied. The experimental results indicated that more than 0.1% C incorporation had a significant inhibitory effect on the out-diffusion of B, but that the inhibition was obviously reduced when the processing temperature was over 1050 °C. In addition, because the atomic radius of C is smaller than that of Si, Ge, the C incorporation compensates the strain of SiGe, and adjusts the lattice mismatch, thus enhancing the thermal stability of SiGe.

1. Introduction
One of the key issues about the NPN SiGe HBT technology is that after the SiGe base epitaxial layer is grown, the narrow-band distribution of boron in the SiGe layer is maintained during the subsequent thermal processes [1]. In the 0.35um or less process technology, an ultra-thin, highly doped SiGe base width is usually only twenty or thirty nm, B dopant in the SiGe base tends to produce out-diffusion in the subsequent processes such as annealing, and so the boron distribution widens or extends to the adjacent Si region, which results in an additional conduction band barrier, and which significantly reduces the device performance [2]. The out-diffusion of boron may be produced by thermal annealing and by transient diffusion enhancement (TED) induced by external implantation/annealing [2]. To solve this problem, the out-diffusion of boron can be suppressed by doping C atom in SiGe layer so as to prevent device performance from degrading [3].

In B-doped SiGe layer, B impurity out-diffusion is carried out through the interstitial displacement mechanism, partial B impurities are changed into the mobile interstitials B atoms (Bi) by replacement reaction (1), and B interstitial Bi moves outward, resulting in the out-diffusion of B impurities.

Bs+I< = >Bi                                                                                      (1)

The diffusion of the C atoms in the SiGe layer is similar to that of the B atom diffusion, and is also caused by displacement reaction between Si self-interstitial atoms. In the region with doping concentration of C higher, substitution reaction between substitutional C atom and self-interstitial Si atom is carried out, as shown in formula (2), which forms a movable interstitial C atom (Ci). The Ci atoms produced by the substitution reaction (2) reduces the number of self-interstitial atoms in the Si, thus reducing the chance of interstitial Bi formation by reaction of B atoms with Si self-interstitials.

Cs+I< = >Ci                                                                                       (2)
As a result, the out-diffusion of C in the region of high C concentration will cause the concentration of undersaturated self-interstitial Si in the C-rich region to decrease, which in turn inhibits the diffusion of boron[4].

2. Experiments and results
The experiment used multilayer structure, as shown in Figure 1, which was deposited by RPCVD (reduced pressure chemical vapor deposition). At first, the 10nm Si buffer was deposited on Si substrate, and then the 35nm undoped SiGe was deposited, followed by 10nm p’ SiGe and 35nm undoped SiGe. P-type doping source used B2H6 for in-situ doping, C was doped in all the SiGe layers, the C source was SiH3CH3, and finally the 10nm Si cap was deposited. The B dopant profile and its change after annealing (B out-diffusion) were characterized by SIMS.

| 10nm Si Cap |
|-------------|
| 35nm SiGe C doping |
| 10nm p+ SiGe C doping |
| 35nm SiGe C doping |
| Si Buffer |
| Si Substrate |

Figure 1. RPCVD-deposited multilayer SiGe sample structure

2.1. Inhibitory effect of different C content on the out-diffusion of B impurity
The first set of experiments was a comparison of the inhibitory effects of different C concentrations on the out-diffusion of B. The content of doped C was 0.1%, 0.2%, and 0.6%, respectively. All the samples were processed under the same annealing conditions at a temperature of 950 °C for 15 minutes. Figure 2 shows the B out-diffusion in sample without C doping after annealing, and apparently B out-diffusion was very serious whose full width at half maximum (FWHM) expanded by 2 times. Figures 3, 4 and 5 indicated the B out-diffusion in the samples with 0.1%, 0.2%, and 0.6% C doped, respectively, after annealing. As can be seen from the figures, the incorporation of 0.1% C has completely inhibited the B out-diffusion, FWHM almost did not expand, while the FWHM of the 0.2% and 0.6% samples roughly expanded by about 5%. 
Figure 2. Sample without C doping

Figure 3. Sample with 0.1% C doped
2.2. B out-diffusion of C doped samples at different annealing temperatures

According to the actual situation of HBT process, 0.1% C-doped samples were annealed at different temperatures, and then the out-diffusion of B was tested. Figure 6. showed annealing at 1000°C for 20s, and there was almost no B out-diffusion in the sample. Figure 7. showed annealing at 1050°C for
20s, and there was about 10% B out-diffusion due to FWHM expansion. When the annealing temperature is 1100 °C with duration 20sec, the out-diffusion of B is up to nearly 200% as result of FWHM expansion, as shown in Figure 8.

![Figure 6. Annealing at 1000°C for 20s](image6)

![Figure 7. Annealing at 1050°C for 20s](image7)
2.3. The strain compensation regulation of C incorporation

X-ray diffraction (XRD) analysis was performed on samples with different C contents. Figure 9 showed the XRD rocking curve of SiGe samples with C content of 0, 0.1%, 0.2% and 0.6%. It can be seen from Fig. 9 that, as the C atom radius is smaller than Si, Ge atom radius, the incorporation of C compensates the lattice mismatch between Si and Ge, and with increase in C doping, the compensation for the strain of SiGe increases.

![Figure 9](image)

**Figure 9.** XRD rocking curve of SiGe samples with C content of 0.1%, 0.2%, 0.6% and 0
3. Conclusions

The inhibitory effect of different C doping on the out-diffusion of B impurity in SiGe and the out-diffusion of B impurity in SiGe at different temperatures were investigated. The results showed that more than 0.1% C incorporation can effectively and fully inhibit the doped B out-diffusion in SiGe in the annealing process. In the process of SiGe HBT devices, the dopant of the emitter was usually activated by rapid thermal annealing. The experiments demonstrated that there was no serious B out-diffusion effect in C-doped SiGe in rapid annealing at 1050°C for 20s. Therefore, incorporation of C greatly improves the heat budget of the process. Meanwhile, as the C atom radius is smaller than Si, Ge atom radius, the incorporation of C compensates the lattice mismatch of SiGe and enhances the thermal stability of SiGe.

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