A Simple Modeling and Simulation of Complete Suppression of Boron Out-Diffusion in $Si_{1-x}Ge_x$ by Carbon Insertion

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Abstract

We present a simple modeling of boron diffusion in $Si_{1-x-y}Ge_xC_y$ by manipulating the strain and the intrinsic carrier concentration. We show that the diffusion of boron is strongly suppressed by a moderate concentration of substitutional C in $Si_{1-x}Ge_x$. This suppression is due to an under saturation of Si self-interstitials in the C-rich region. The results obtained from the proposed model are in good agreement with the measured values.

1. Introduction

The integration of SiGe alloy layers has opened the possibility of combining advanced Si microelectronics technology with the unique advantages of heterostructure devices. A prominent example for this exploitation of bandgap engineering is the heterojunction bipolar transistor (HBT). A key problem in npn SiGe HBT technology is retaining the narrow as-grown boron profile within the SiGe layer during post-epitaxial processing. However, boron diffusion into the Si region during device processing causes undesirable conduction band barriers, and thus significantly degrades device performance. Boron out-diffusion can be caused by: (1) thermal annealing, (2) transient enhanced diffusion (TED) due to an extrinsic boron implantation and anneals etc., An additional degree of freedom of the fabrication process is given by adding substitutional C in SiGe HBTs as a further diffusion suppressing agent [1]. The suppression of B diffusion due to Ge and C allows the control of steep doping profiles during device processing. Addition of C has also the advantage that it reduces the misfit strain and eliminates secondary defects at the amorphous/crystal (a/c) interface in ion-implanted Si was proposed by Nishikawa et al. [2]. The present modeling and simulation suggests that substantially higher thermal budgets can be tolerated when substitutional carbon in concentrations of the order of 0.1 atomic % is added to the SiGe layer [1]. We show that the strong suppression of B diffusion can be achieved by a small amount ($\sim 10^{20}$ cm^{-3}) of substitutional C in SiGe.

2. Model

Diffusion of C out of regions with higher C concentrations can cause localized under saturation of Si self-interstitials in the C rich region, which, in turn, results in suppressed diffusion of boron. Mobile interstitial carbon atoms (C_I) are created through the reaction of Si self-interstitials (I) with immobile substitutional carbon (C_s):

$$C_s + I \Leftrightarrow C_I \qquad (1)$$

The formation of C_I pairs through the replacement reaction of Eq. (1) reduces the amount of interstitials available for pairing with substitutional B, thereby lowering the B diffusivity. The boron impurity flux is given as [3-4]:

$$J_B = -D_B \Psi \left(\frac{\partial C_B}{\partial x} + \frac{C_B}{Q}\frac{\partial N_T}{\partial x} + \frac{2C_B n}{Q}\frac{\partial \ln n_i}{\partial x} \right) \quad (2)$$

Ψ allows for the concentration dependence of D_B.
The boron diffusivity is modeled in a simplified form as follows:

$$D_B = \left(\frac{C_I}{C_I^*} \right) \Psi D_{B0} \exp(-E_A / kT) \quad (3)$$

where D_{B0} is the pre-exponential factor for the diffusivity. Here, the boron diffusivity includes the effect of Si interstitials, because it is proportional to the ratio between the concentration of Si interstitial C_I and the equilibrium concentration of Si interstitial C_I^*. E_A is the activation energy of B in Si, which is modified to fit for $Si_{1-x-y}Ge_xC_y$ is: $E_A = 3.62 + (0.4.x.y) \pm 0.0154$, where x and y are at. % fractional values of germanium and carbon respectively. According to the Eqs. (2) and (3), the retardation of B diffusion in the C implanted sample may be attributed to the deactivation of B, which leads to a lower hole concentration p. The addition of C in $Si_{1-x}Ge_x$ has been used for strain compensation [1]. At certain Ge and C levels, the strain due to Ge and C atoms becomes important for the boron diffusivity in $Si_{1-x-y}Ge_xC_y$. So, the boron diffusivity, given in Eq. (3) can be modified by multiplying with exp(-fS/kT). Here S is the local strain due to the presence of Ge and C and defined as: $S = |S_{Ge} - S_C|$; $S_{Ge} = \delta \cdot x ; S_C = R\delta \cdot y$, where δ is the moderate lattice mismatch between Si and Ge (~0.042), R is the strain compensation ratio (~10.71) [1], and f is the activation energy per unit strain, which is modified as: $f \rightarrow (f' - 0.4 * x * 100)$. The bandgap difference (ΔE_g) between $Si_{1-x}Ge_x$ and $Si_{1-x-y}Ge_xC_y$ is supposed to affect intrinsic carrier concentration n_i and results in the difference in D_B as well as in boron flux in Eq. (2). The intrinsic carrier concentration as a function of temperature is given by: $n_i^{SiGeC} = \sqrt{(N_C N_V)^{SiGeC}} \exp(-(E_g + \Delta E_g)/2kT)$ where N_C and N_V are the effective density of states in the conduction and valence bands for SiGeC and $\Delta E_g = E_{gsT} + (E_{grT} - E_{gsT})(1 - F_{pm})$. Here E_{gsT} is the energy gap due to strain, is approximated by $E_{gsT} = x(0.767 + (1.71/R))$.

Since B diffusion is primarily attributed to an interstitials mechanism, it is retarded if the concentration of interstitials C_I is reduced as compared to the equilibrium value C_I^*. To examine this point, we simulated the B diffusion in $Si_{1-x-y}Ge_xC_y$ by using the process and device simulator TAURUS through Physical Model and Equation Interface (PMEI) [4]. Since we assumed that C_I is equal to C_I^*, the change in boron diffusivity defined in the Eqs. 2-3 should be a measure of C_I averaged around the boron diffusion region. We changed the value of pre-factor D_{Bo} and by the inclusion of models for the modified activation energy of B (which includes the strain with f factor) and intrinsic carrier concentration for $Si_{1-x-y}Ge_xC_y$ to fit the simulated profile to the experimental one as discussed below.

3. Results and discussion

Fig. 1 shows the SIMS as-grown and annealed profiles of boron spikes and C with peak concentration of $5x10^{19}$ cm^{-3} (0.1 at. %), as well as the profiles from the

present model. Nearly four peaks of B spikes were incorporated in the C-rich regions, and in the adjacent region without interstitial C doping. We found strongly enhanced diffusion of B spikes in the C- poor region. The suppression of B diffusion at high C

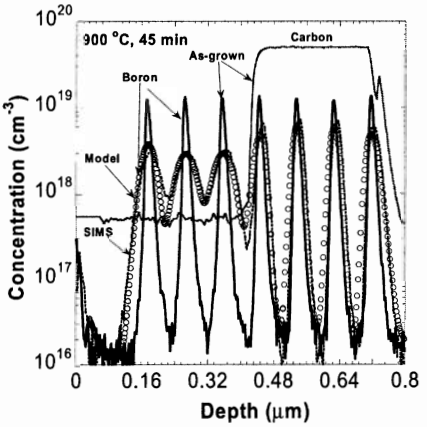

Fig.1 Comparison of SIMS with simulation for C: $5x10^{19}$ cm^{-3}. Open circules and dotted lines are after anneal from simulation and SIMS. SIMS profile are from Rucker et al. [5].

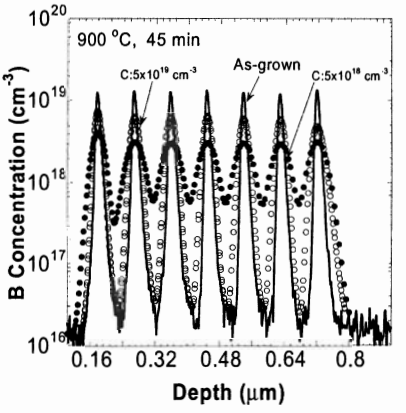

Fig.2 Depth profiles of B with different background C conc. Solid line is the as-grown and symbols are the annealed samples after 900 °C, 45 min.

concentrations are consistent with the under-saturation of Si self-interstitials in the C-rich region predicted by theory from Rucker et al. [5]. The profiles obtained from the present model agree very well with the experimental profiles in both C-poor and rich regions. The deduced D_{B0} for the sample with a C concentration of $5x10^{19}$ cm^{-3} was 0.159 cm^2/s, which is obviously smaller than the reported value for Si [2] as well as for $Si_{1-x-y}Ge_xC_y$ [1] due to the inclusion of models for strain and n_i. Fig.2 shows the dependence of TED suppression by various C concentrations (at the background) for three B doping super-lattices. It has been reported that TED of boron is strongly suppressed in C-rich Si [1]. The calculated B profile in the C-poor sample shows strongly enhanced diffusion of B. The calculated results agree well with the measurement, as well as with those reported by Rucker et al. [5]. We conclude from the present simulation and measurement [5] that TED of B is suppressed in adjacent regions of low C concentrations.

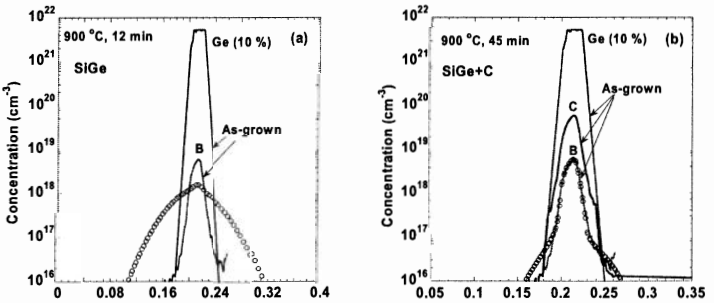

Fig.3 Depth profiles of B, Ge and C as-grown and B (open circles) after anneal at 900 °C, 12 min without carbon (a) and with carbon after anneal at 900 °C, 45min (b).

Figs. 3(a) and (b) show the measured as-grown and the annealed simulated results without and with C respectively, which demonstrate that the boron is confined well within the SiGe (or SiGeC) layers. The layered structure without C exhibits strong boron out-diffusion. Fig. 4 shows the intrinsic boron diffusivity D_B that was

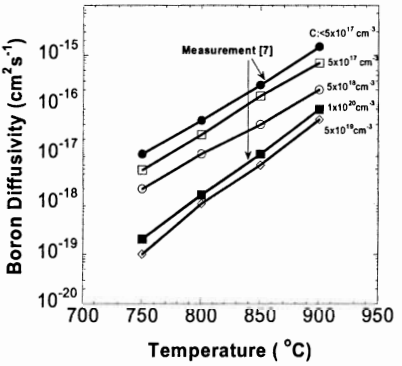

Fig.4 Intrinsic B diffusivity as a function of annealing temperature for three C concentration. Measurement values are also given in the plot.

determined as a function of C concentration and annealing temperatures from the measurement [5], and from the present simulation. For increasing C concentrations, we find a strong suppression of the B diffusivity by a factor, which is almost independent of temperature.

4. Conclusion

We have developed a model for the diffusion of boron in $Si_{1-x-y}Ge_xC_y$ that is based on the modification of the strain, intrinsic carrier concentration and band gap narrowing. We have demonstrated that the diffusivity of boron is strongly suppressed by high concentrations of substitutional C. This observation is interpreted in terms of an under-saturation of Si self-interstitials in the C-rich region. Finally, we have shown that the results from the present simulation agree well with the measurement values.

References

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