Measurement and Simulation of Boron Diffusivity in Strained $\text{Si}_{1-x}\text{Ge}_x$ Epitaxial Layers

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Diffusion of boron in compressively strained $\text{Si}_{1-x}\text{Ge}_x$ alloy layers grown by rapid pressure chemical vapor deposition has been studied as a function of the composition for $0.0006 \leq x \leq 0.15$ and annealing temperature. The comparison of the $\text{Si}_{1-x}\text{Ge}_x$ samples to the Si samples after rapid thermal and furnace annealing revealed a retarded B diffusion inside the strained $\text{Si}_{1-x}\text{Ge}_x$ layers. The influence of the Ge content on the dopant diffusion was also measured and simulated, demonstrating that the diffusion of B was found to decrease with the Ge alloy content and annealing temperature. A simple empirical expression for the B retardation is presented and incorporated into a diffusion model for dopants in heterostructures. Good agreement between the measured and simulated diffusivity that includes the model for strain and chemical effects are obtained. By comparing with experimental values, our extracted (by using experiment and simulation) B diffusivity predicted a lower value (retardation).

Keywords: SiGe; Boron; Simulation; Diffusivity; RTA; Furnace anneal

1. INTRODUCTION

Silicon Germanium (SiGe) HBT BiCMOS is a new promising technology that offers the possibility of integrating very high performance HBTs with state-of-the-art CMOS. Diffusion of dopants in a crystalline Si and Ge is an example where controlled experiments in pristine material have led to complex, phenomenological models. These models, although limited in their absolute prediction of diffusivity, do provide a guide for predicting the change of diffusivity with certain material properties including Ge fractions,

chemical effects *etc.*, and physical parameters including temperature *etc.* Retarded B diffusion has been observed in compressively strained $\text{Si}_{1-x}\text{Ge}_x$ alloys [1]. Some confusion has existed about the origin of this retardation. Moriya *et al.* [2] and Cowern *et al.* [3] compared the diffusion in strained SiGe with that in relaxed Si and thus neglected any chemical effects. Recently Kuo *et al.* [4] have made a detailed comparison of the B diffusion in compressively strained SiGe with that in relaxed SiGe of the same composition and in tensile-strained Si with that in relaxed Si. They find no effect from the strain on the diffusivity.

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These observations disagree with the total energy calculation [5] of the formation energies of the self-interstitial and the vacancy in compressive and tensile-strained silicon. The calculations show that the formation energy of the self-interstitial increases with increasing compressive strain and decreases with increasing tensile strain.

A simple and accurate empirical diffusion model that fits for various Ge concentrations and thermal budget is developed and implemented in a TAURUS-PMEI (Physical Model and Equation Interface) [6]. The present diffusion model accurately simulates the measurement profiles over the given range of Ge fractions, and box-type and graded Ge profiles that were selected as experimental conditions involved in the present study. In this paper, we have made a detailed investigation of the diffusion of B in compressive strained $\text{Si}_{1-x}\text{Ge}_x$ at different Ge content (x (%): 0.06, 0.2, 4, 10 and 15) as a function of temperature, and Ge fractions. The simulated and measured results are in good agreement with other reports [7] and experimental results [1–2, 4] such that we consider them as a very important factor for the process design of $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$ heterostructure devices. With the present models and simulations it has been possible for the first time to the knowledge of the authors to separate chemical effects (alloy effect) as well as strain (with f factor) from effects arising from strain in interstitial-mediated diffusion of B in strained $\text{Si}_{1-x}\text{Ge}_x$ epitaxial layers.

2. EXPERIMENTAL DESIGN

The aim of the experiment carried out in the present study is to provide experimental data needed for the calibration of the present model. The SiGe layers have been grown in an ASM Epsilon 2000 RPCVD single wafer reactor. The Si cap/ $\text{Si}_{1-x}\text{Ge}_x$ layer/Si spacer stack was grown epitaxially on p-Si (100) substrates for five different Ge fractions as mentioned above as well

as graded Ge profiles. The samples were grown with target box B profiles with doping concentrations of $5 \times 10^{18} \text{ cm}^{-3}$. Samples with boron box profiles in the Si-capping layer, $\text{Si}_{1-x}\text{Ge}_x$ epitaxial layer and Si spacer have been studied. The samples with the box-type Ge profiles were submitted to thermal budgets (furnace anneal) ranging from 850°C for 20 min, 850°C for 60 min, 900°C for 4 min and 900°C for 12 min. The samples with graded type Ge profile were submitted to the following thermal budgets: rapid thermal annealing (RTA) are at 900°C, 950°C, 1050°C and 1100°C each for 10 sec, and furnace anneal (FA) are at 850°C for 20 min followed by the RTA at 900°C, 950°C 1000°C and 1100°C each for 10 sec.

3. DIFFUSION MODEL

The boron impurity flux is given by [8, 9]:

$$J_B = -D_B \psi \left(\frac{\partial C_B}{\partial x} + \frac{C_B}{Q} \frac{\partial N_T}{\partial x} + \frac{2C_B n}{Q} \frac{\partial \ln n_i}{\partial x} \right) \quad (1)$$

where $Q = \sqrt{(N_T^2 + 4n_i^2)} = n + p$ and $\psi = ((1 + \beta(p/n_i))/(1 + \beta))$ allows for the inclusion of the concentration dependence of the effective diffusion coefficient. D_B is the boron diffusivity, C_B is the boron concentration, N_T is the net doping ($N_A \sim N_D$), n is the electron concentration and n_i is the intrinsic carrier concentration for SiGe.

The boron diffusivity is modeled in a simplified form:

$$D_B = \psi D_{B0} \exp(-E_A/kT) \quad (2)$$

where D_{B0} is the pre-exponential factor for the diffusivity, E_A is the activation energy for Si, which is modified as: $E_A = 2.87 + (0.015 * x * 100)$ where x is the Ge fraction.

At certain Ge content, the strain due to Ge atoms becomes important for the boron

diffusivity:

$$D_B = \psi D_{B0} \exp(-E_A/kT) \exp(-fS/kT) \quad (3)$$

where S is the local strain due to the Ge as well as B presence: $S = S_{Ge} + S_B$. After substituting the constants of B and Ge, it becomes: $S = 0.0425c_{Ge} - 0.274c_B$ where c_{Ge} and c_B are the atomic fraction of Ge and B in Si respectively. f is the activation energy per unit strain is modified to: $f' = 0.4 \times 100$ where f' is given by [3]

$$f' = -\frac{kT}{X} \ln\left(\frac{\hat{D}}{D}\right) \quad (4)$$

and $\hat{D}$ and D are the diffusivity in the strained material and the corresponding diffusivity in the unstrained material, respectively.

The intrinsic carrier concentration as a function of temperature is given by: $n_i(\text{SiGe}) = n_i(\text{Si}) \exp(-E_g/2kT)$.

In addition there is a trapping of B atoms with Ge atoms and the complex Ge-B acts as a clustering center for the B clusterisation process to transfer B atom into the electrically inactive entities. Because of this chemical or trapping effect, the change in the boron diffusivity is given by: $D_{B\text{eff}} = -D_B(1/(1 + C_{Ge}/C_{ch}))$ where c_{Ge} and c_{ch} are the Ge and characteristics concentrations, respectively.

4. RESULTS AND DISCUSSION

Figure 1 shows the comparative analysis of the present simulation results with SIMS for the Ge with fractions of 10% and thermal budgets at 850°C for 60 min. It appears that the calculated and SIMS diffused profiles fit very well. This shows that the reduction of the B concentration in the underlying Si substrate and $\text{Si}_x\text{Ge}_{1-x}/\text{Si}$ is caused by the reduction of the effective B diffusivity in the $\text{Si}_x\text{Ge}_{1-x}/\text{Si}$ interface region. The SIMS of the B initial as-grown profiles are

FIGURE 1 Comparison of simulation to the SIMS profile of a sample of 10% Ge, $3 \times 10^{18} \text{ cm}^{-3}$ B at 850°C for 60 min. The model and the SIMS results are after the above mentioned thermal budget.

given in Figure 1, which shows that the different B peaks were studied. The starting point for the simulation consists of the as-grown profiles of Ge and B, extracted from the SIMS measurements. Figure 2 shows the B diffusivity as a function of reciprocal temperature for various Ge contents. Notice that the 10% and 15% Ge samples are distinctly different from 0% and 0.2% Ge samples. By comparison with experimental values, our model results that include the strain and chemical effects show very much retardation of boron diffusivity with Ge fractions. The dependence of temperature, obtained from this plot for the boron diffusivity is: $3 \times 10^{-3} \exp(-3.07489/kT) \text{ cm}^2/\text{sec}$ at 10% Ge fractions. The relative diffusivity of B in the different layer, extracted by using the present model as well from the experiments are shown in Figures 3(a) and 3(b). Figure 3(a) illustrates the strong dependence of the dopant redistribution on the Ge content in the strained layers. It shows that boron diffusivity reduce more rapidly until Ge is 10%, then it seems to be slow and saturate as predicted experimentally by Moriya *et al.* [2]. Here, it is interesting to note that

FIGURE 2 Extracted Boron diffusivity as a function of the reciprocal temperature for Ge content from 0.06% to 15%. Experimental [1] and Monte-Carlo simulation [10] results are also plotted. (*) Results from the present model. From the Ref. [1], Ge with 0% and 10% have different thermal budgets. M-C simulation results are from the Ref. [10].

perfect coincidence of the model and the experimental B diffusivity irrespective of any type of thermal budgets. The overlapping of some of the sample values are due to the extraction of B as well as the Ge peaks after the thermal budgets, which have different types of as-grown samples (peaks). Figure 3(b) shows the comparison of boron diffusivity (of both box-type and graded type Ge profiles) with the experimental values. Our extracted results of graded Ge profile shows very much retardation of B diffusivity at high annealing temperature, irrespective of RTA or FA or the combination of both. It is argued that B diffusion in strained SiGe layers requires the inclusion of both the strain and the chemical effects. By comparing with experimental values, our extracted (by using experiment and simulation) B diffusivity predicted a lower value (retardation). The influence of FA after RTA on B diffusivity has only a marginal effect.

FIGURE 3 (a) Extracted and experimental boron diffusivity as a function of Ge fraction with different thermal budgets for the RPCVD grown multilayer structure with different Ge contents in each layer. Also shown are the experimental values from Kuo *et al.* [4, 11] and Moriya *et al.* [2]; (b) Same as above with annealing temperatures including RTA and RTA + FA. Comparison with other experimental results are also given.

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