

Simulation of Boron Diffusion in Strained Si_{1-x}Ge_x Epitaxial Layers

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Abstract: This paper describes a simple and accurate model for boron diffusion in SiGe that was successfully implemented in TAURUS (PMEI). The comparison of the Si_{1-x}Ge_x samples to the Si samples after rapid thermal and furnace annealing revealed a retarded B diffusion inside the strained Si_{1-x}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. The model fits for various Ge % (both box and graded profiles) and thermal budgets. The simulation results of various Ge % and thermal budgets show good agreement with measurement data and the predicted B diffusivity show a reasonably low value.

I. 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. The device performance is improved by utilizing the material properties of Si_{1-x}Ge_x. The ability to increase the doping in the base without degrading the emitter junction efficiency is one of the major advantages of the SiGe HBT. However, the high doping concentration and the grading of the Ge composition in the base layer, associated with high performance Si_{1-x}Ge_x layer, can make it difficult to predict the out-diffusion of Boron (B) from the Si_{1-x}Ge_x layer. Hence, an understanding of the diffusion of B in a SiGe alloy film is important. We have studied the B diffusion in Si_{1-x}Ge_x with box-type germanium (Ge) concentration fraction x : 0.02%, 0.6%, 4%, 10% and 15% and graded-type Ge with *in situ* doped epitaxial layers with B concentrations at three depths under the various Thermal Budgets (TB) using SIMS. A simple and accurate empirical diffusion model that fits for various Ge concentrations and TB is developed and implemented in a TAURUS-PMEI (Physical Model and Equation Interface)[1]. The present diffusion model accurately simulates the measurement profiles over the range of Ge concentrations, and box and graded Ge profiles that were selected as experimental conditions involved in the study.

II. 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/Si_{1-x}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, Si_{1-x}Ge_x and Si spacer have been studied.

III. DIFFUSION MODEL

The present diffusion model is essentially a modified model of Lever et al [2], with the inclusion of the strain dependence of the activation energy of the diffusion coefficient [3]. Also the model for intrinsic carrier concentration of SiGe, drift field due to band-gap narrowing, modified strain model which includes the strain due to the fractions of Ge concentration (c_{Ge}) and also the boron concentration (c_B) are included [4]. The B flux, J_B is given by

$$J_B = -D_B^0 \psi \left(\frac{\partial C_B}{\partial x} + \frac{C_B}{Q} \frac{\partial N_T}{\partial x} + \frac{2C_B n}{Q} \frac{\partial \ln n_i}{\partial x} \right) \quad (1)$$

where $Q = \sqrt{N_T^2 + 4n_i^2} = n + p$

and N_T is the net doping, n is the electron concentration and n_i is the intrinsic carrier concentration. C_B is the boron concentration, ψ models the concentration dependence of the effective diffusion coefficient, p is the hole concentration, and D_B^0 is the B diffusivity.

(a) *Strain in SiGe:* The generalized total strain, s , due to the superposition of the strain s_B , attributed to the presence of B and the strain s_{Ge} , attributed to the presence of Ge, is involved in the compensation theory [3]:

$$s = s_B + s_{Ge} = 0.0425c_{Ge} - 0.274c_B \quad (2)$$

(b) *Trapping of B with Ge:* Determining the nature of Ge concentration dependence of the B diffusivity is the primary focus of this work. In the presence of isovalent atoms like Ge, which act as traps for B atoms, the complex Ge-B acts as a center for the B clustering process. Due to this trapping, the (effective) boron diffusivity from eqn.(1) is:

$$D_{B_{eff}} = D_B^0 \frac{1}{1 + (C_{Ge} / C_{ch})} \quad (3)$$

C_{Ge} and C_{ch} are the Ge and characteristics concentrations respectively. It is note this formula has a non-singular asymptotic behaviour so that when $C_{Ge} \rightarrow 0$ then $D_{Beff} \rightarrow D_B$. This is more consistent behaviour than the one described by the above Eq.(3).

(c) *Intrinsic carrier concentration:* In the case of graded or even box-like Ge profile in an HBT structure is used, the result is a position dependence of the intrinsic mobile charge carrier concentration and the appearance of the electric field $E_b \propto \nabla n_i$. It should be noted that there is no off-the-shelf model. The interpolation between the Si and Ge descriptions can not be used because the Si indirect band-gap is between the top of the valence band and the bottom of the Δ -conduction band whereas the Ge indirect band-gap is between the top of the valence band and the bottom of the L-conduction band.

$$n_i = \sqrt{N_C N_V} \exp(-\Delta E_g / 2kT) \quad (4)$$

where, N_C and N_V are the effective density of states in the conduction band and valence band, and ΔE_g is the band gap between Si and SiGe and depends on the Ge fraction, temperature etc.

(d) *Boron diffusivity in SiGe:* The boron diffusivity is modeled in a simplified form:

$$D_B = \Psi D_{B0} \exp(-E_A / kT) \quad (5)$$

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:

$$D_B = \Psi D_{B0} \exp(-E_A / kT) * \exp(-fS / kT) \quad (6)$$

where f is the activation energy per unit strain is modified to: $f' = -0.4 * x * 100$ where f' is given by:

$$f' = -\frac{kT}{S} \ln\left(\frac{\hat{D}}{D}\right) \quad (7)$$

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

IV. RESULTS AND DISCUSSION

The simulations were performed in a recently available simulation package TAURUS [4] through physical model and equation interface (PMEI). Fig.1 shows the calculated and measured profiles of for the box-type Ge with fractions and.

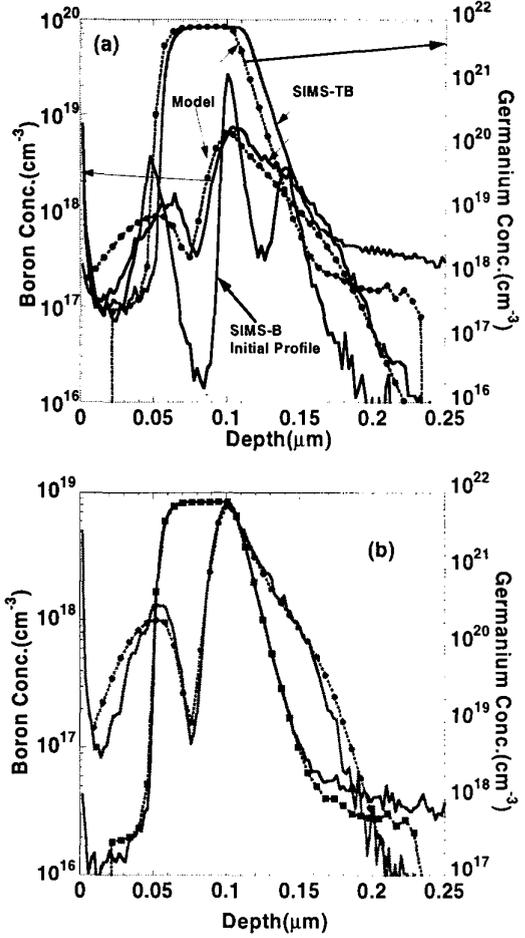


Fig.1 Comparison of simulation with SIMS diffusion profile of Box-type Ge profile with 15% Ge. (a) 850° C, 60 min; (b) 900° C, 12 min

thermal budgets are (a) 15%, 850 °C, 60 min and (b) 15%, 900 °C, 12 min. It appears that the calculated and SIMS diffused profiles fit very well and the diffusivity of B decreases with the increase of Ge content. This shows that the reduction of the B concentration in the underlying Si substrate of $Si_{1-x}Ge_x/Si$ is caused by the reduction of the effective B diffusivity in the $Si_{1-x}Ge_x/Si$ interface region. Fig.2 shows the simulated and measured profiles of graded-Ge profile for the Rapid thermal annealing (RTA) are (a) 1100 °C for 10 sec and (b) Furnace annealing (850 °C/20 min and RTA (900 °C/10 sec). It is interesting to note that the simulated and SIMS diffused profiles fit very well and the diffusivity of B increases with the increase of annealing temperature. In the case of lowering annealing time, the B concentration in the $Si_{1-x}Ge_x$ layer become higher than the B concentration in Si. This phenomena is due to the decrease of B atoms that have redistributed from $Si_{1-x}Ge_x$ layer to the Si substrate. For some of the thermal budgets the diffusion of B in strained $Si_{1-x}Ge_x$ resulted into diffusion into the relaxed Si layers on both sides of the diffused profiles as given in the above figures.

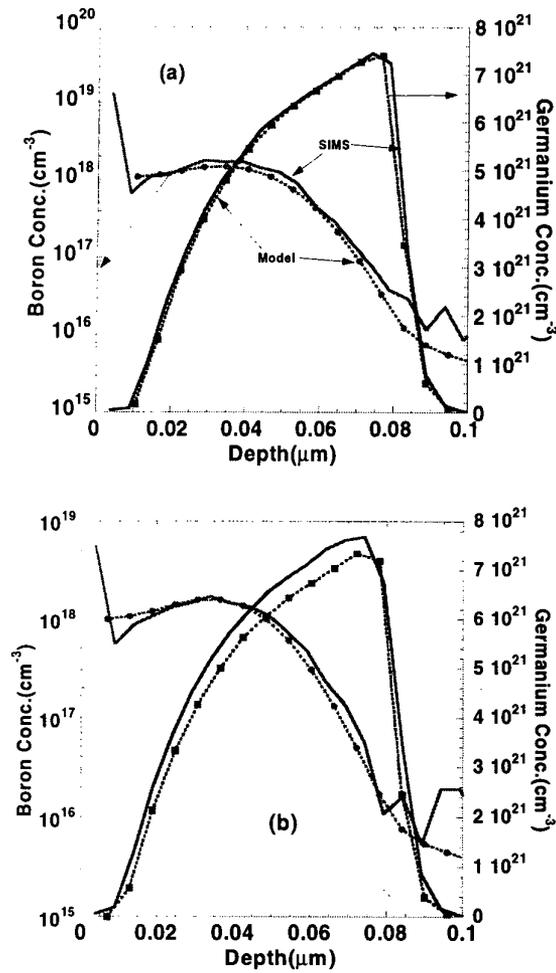


Fig.2. Similar to Fig.1 with Ge:15% (Ge-graded profile).
 (a) Rapid Thermal Annealing(RTA): (1100°C, 10sec);
 (b) Furnace Annealing (FA)&RTA : (850° C/20min & 900° C/10sec)

Fig.3 (a) shows the calculated as well as extracted boron diffusivity from simulation and experiment with different thermal budgets as a function of Ge fraction. As for the diffusion analysis in the $Si_{1-x}Ge_x$ layers, we have simulated or calculated the diffusion profile using the band-gap modified diffusivity approach as a function of temperature and Ge content. The intrinsic diffusivity and band-gap change were assumed to be different at each layer with Ge content. The relative diffusivity of boron in the different layer, extracted by using the present model as well as from the experiments are shown. This illustrates the strong dependence of the dopant redistribution on the Ge content in the strained alloys. It shows that boron diffusivity reduces more rapidly until Ge is 10%, when it seems to be slow and saturates as predicted experimentally by Moriya et al. [7]. Here, it is interesting to note a perfect coincidence of the model and the experimental B diffusivity irrespective of any type of thermal budgets. The overlap of some of the sample values are due to the extraction

of B as well as Ge peaks after the thermal budgets, which have types of as-grown sample (peaks).

Fig.3 (b) shows the extracted B diffusivity as a function of annealing temperature. The experimental values of 0-15 % Ge fractions at 950 °C [9], 17 % and 18 % of Ge at 800 °C and 860 °C [5,6] and 30 % Ge at the range of annealing temperature between 850 °C to 1000 °C [7] are also given. The 24 % of Ge at the annealing temperature ranges between 825 °C to 850 °C are plotted along with the extracted results [10]. It is noted that higher Ge samples distinctly differ from 0 % and 5 % Ge samples. By comparison with the experimental values, our extracted results of graded Ge profile shows very much retardation of B diffusivity at higher

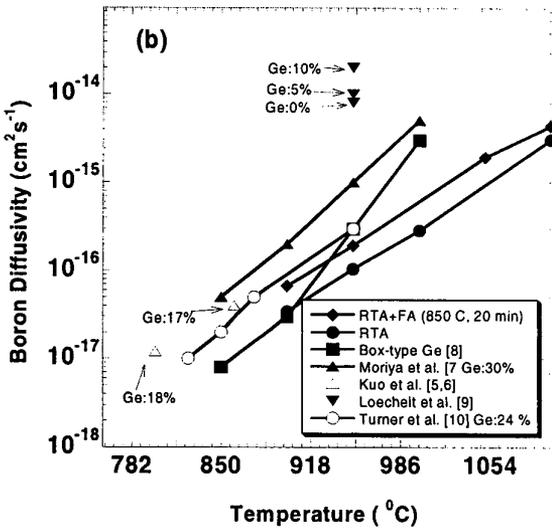
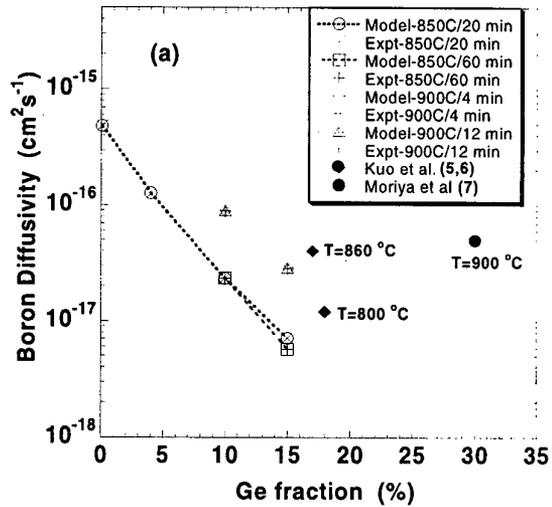


Fig.3 Extracted B diffusivity as a function of (a) Ge-fraction and (b) Temperature.

annealing temperatures, irrespective of RTA or FA or the combination of both. The dependence of temperature obtained from this plot for the B diffusivity are in good agreement with M-C [11] simulation as well as from different experimental observations [12]. It is interesting to note that our extracted results show a lower value of the boron diffusivity compared to the available values [2-7, 10-12]. It is to be estimated that the boron diffusivity in $\text{Si}_{0.85}\text{Ge}_{0.15}$ is nearly two orders of magnitude less compare to Si at 925 °C for 20 min [11].

V. CONCLUSIONS

A simple and accurate model describing the B diffusion in strained SiGe is successfully implemented in TAURUS through Physical Model and Equation Interface (PMEI). The simulation results of both B and Ge diffusion profiles with various Ge percentages and thermal budgets are in good agreement with the measured data. The influence of FA after RTA has only a marginal effect on B diffusion. Based on the available experimental values, the present extracted B diffusivity predicted a lower value and found retarded B diffusion inside the strained SiGe layers compare to Si part. The good agreement between the measured and simulated B diffusivity and Si-Ge inter-diffusion has been observed. It has been argued that B diffusion in strained SiGe layers requires the inclusion of both the trapping effect as well as the strain in the formulation of the diffusion mechanism.

ACKNOWLEDGEMENT

The authors wishes to acknowledge Milan Libezny and V.I. Kold'yaev for the useful discussions. Part of this was work performed in the frame work of the MEDEA T555 project. Authors also acknowledge W. Vandervorst for the SIMS data.

REFERENCES

1. Taurus Process/Device, Ver. 98.4, Avant! Corp, USA.
2. R.F. Lever, J.M. Bonar, and A.F.W. Willoughby, "Boron diffusion across silicon-silicon germanium boundaries," *J. Appl. Phys.*, vol. 83, pp. 1988-1994, Feb. 1998.
3. N.E.B. Cowern, P.C. Zalm, P. Vander Sluis, D.J. Gravesteijn, and W.B. de Boer, "Diffusion in strained (SiGe)", *Phys. Rev. Lett.*, vol. 72, pp. 2585-2588, April 1994.
4. V.I. Kol'dyaev, "Models for the B, As, Ge and P diffusion in a strained HBT structure suitable for TCAD applications," IMEC internal report, pp. 1-35, March 1998.
5. P. Kuo, J.L. Hoyt, J.F. Gibbons, J.E. Turner and D. Lefforge, "Effects of strain on boron diffusion in Si and $\text{Si}_{1-x}\text{Ge}_x$," *Appl. Phys. Lett.*, vol. 66, pp. 580-582, Jan. 1995.
6. P. Kuo, J.L. Hoyt, J.F. Gibbons, J.E. Turner, R.D. Jacowitz and T.I. Kamins, "Comparison of boron diffusion in Si and strained $\text{Si}_{1-x}\text{Ge}_x$ epitaxial layers," *Appl. Phys. Lett.*, vol. 62, pp. 612-614, Feb. 1993.
7. N. Moriya, L.C. Feldman, H.S. Luftman, C.A. King, J. Bevk, and B. Freer, "Boron diffusion in $\text{Si}_{1-x}\text{Ge}_x$ epitaxial layers," *Phys. Rev. Lett.*, vol. 71, pp. 883-8836, August 1993.
8. K. Rajendran and W. Schoenmaker, "Simulation of Boron Diffusivity in Strained $\text{Si}_{1-x}\text{Ge}_x$ Epitaxial Layers," Submitted to *J. Appl. Phys.*, Jan. 2000.
K. Rajendran, S. Decoutere, W. Schoenmaker, R. Loo, M. Caymax and V. Vandervorst, "Measurement and simulation of boron diffusion in strained $\text{Si}_{1-x}\text{Ge}_x$ epitaxial layers," Submitted to *IEEE Trans. on Elect. Devices*, Jan. 2000.
9. G.H. Loechelt, G. Tam, J.W. Steele, K.K. Knoch, K.M. Klein, J.K. Watanabe and J.W. Christiansen, "Measurement and simulation of boron diffusion in Si and strained $\text{Si}_{1-x}\text{Ge}_x$ epitaxial layers during rapid thermal annealing," *J. Appl. Phys.*, vol. 74, pp. 5520-5526, Nov. 1993.
10. J.E. Turner, T.I. Kanuins, M.P. Scott, H.Y. Keller, "Method of fabricating an ultra-thin active region for high speed semiconductor devices," US Patent No. US5177025, Jan.5 1993.
11. M.J. Caturla, "Toward predictive atomistic model of ion implantation and dopant diffusion in silicon," *Computational Mat. Sci.*, vol. 12, pp. 319-332, March 1998.
12. A.S. Solm and F. Baruffaldi, *J. Appl. Phys.* Vol. 69, pp. 2135-2140, Dec. 1991.