ELSEVIER

Materials Science and Engineering B 124–125 (2005) 39–44

MATERIALS SCIENCE & ENGINEERING B

www.elsevier.com/locate/mseb

Boron diffusion in strained and strain-relaxed SiGe

C.C. Wang [a,*], Y.M. Sheu [a], Sally Liu [a], R. Duffy [b], A. Heringa [b], N.E.B. Cowern [c], P.B. Griffin [d]

[a] *Device Engineering Division, R&D, Taiwan Semiconductor Manufacturing Company, Hsin-Chu 300-77, Taiwan, ROC*
[b] *Philips Research Leuven, Kapeldreef 75, 3001 Leuven, Belgium*
[c] *Advanced Technology Institute, University of Surrey, Guildford, Surrey GU2 7XH, UK*
[d] *Center for Integrated Systems, Stanford University, Stanford, CA 94305, USA*

Abstract

SiGe has been utilized for aggressive CMOS technologies development recently and there are many references [M. Shima, T. Ueno, T. Kumise, H. Shido, Y. Sakuma, S. Nakamura, Symposium on VLSI Technology Technical Digest, 2002, pp. 94–95; T. Ghani, M. Armstrong, C. Auth, M. Bost, P. Charvat, G. Glass, T. Hoffmann, K. Johnson, C. Kenyon, J. Klaus, B. McIntyre, K. Mistry, A. Murthy, J. Sandford, M. Silberstein, S. Sivakumar, P. Smith, K. Zawadzki, S. Thompson, M. Bohr, International Electron Devices Meeting Technical Digest, December 2003, pp. 978–980; P. Bai, C. Auth, S. Balakrishnan, M. Bost, R. Brain, V. Chikarmane, R. Heussner, M. Hussein, J. Hwang, D. Ingerly, R. James, J. Jeong, C. Kenyon, E. Lee, S. Lee, N. Lindert, M. Liu, Z. Ma, T. Marieb, A. Murthy, R. Nagisetty, S. Natarajan, J. Neirynck, A. Ott, C. Parker, J. Sebastian, R. Shaheed, S. Sivakumar, J. Steigerwald, S. Tyagi, C. Weber, B. Woolery, A. Yeoh, K. Zhang, M. Bohr, International Electron Devices Meeting Technical Digest, December 2004, pp. 657–660] presenting the advantages brought by it. A better understanding regarding the boron diffusion behavior within and in the vicinity of SiGe is necessary to optimize the extension and the source/drain in pMOSFET. In order to achieve the goal, both effects from mechanical strain and Ge doping on boron diffusion have been investigated. However, only a few publications discuss the impacts of both. Furthermore, most researches investigate these two effects under the conditions of low boron concentration [P. Kuo, J.L. Hoyt, J.F. Gibbons, J.E. Turner, D. Lefforge, Appl. Phys. Lett. 66 (January (5)) (1995) 580–582; N.R. Zangenberg, J. Fage-Pedersen, J. Lundsgaard Hansen, A. Nylandsted Larsen, J. Appl. Phys. 94 (September (6)) (2003) 3883–3890] and high thermal budget anneal [P. Kuo, J.L. Hoyt, J.F. Gibbons, J.E. Turner, D. Lefforge, Appl. Phys. Lett. 66 (January (5)) (1995) 580–582; N.R. Zangenberg, J. Fage-Pedersen, J. Lundsgaard Hansen, A. Nylandsted Larsen, J. Appl. Phys. 94 (September (6)) (2003) 3883–3890; S. Eguchi, C.N. Chleirigh, O.O. Olubuyide, J.L. Hoyt, Appl. Phys. Lett. 84 (January (3)) (2004) 368–370] in which the equilibrium state of point defects is achieved. These are not the conditions used in aggressive CMOS technologies. Our experiment has therefore been designed to investigate boron diffusion in both strained and strain-relaxed SiGe including ultra-low energy, high concentration boron implant and spike RTA. Models are proposed and the retardation factors corresponding to Ge concentration and stress effect were successfully extracted through these experiments. This paper describes these experiments, with the calibration and the resulting diffusion constants for an ultra-shallow boron junction in SiGe that is popular in advanced CMOS technology.
© 2005 Elsevier B.V. All rights reserved.

Keywords: Boron diffusion; CMOS technology; Strain-relaxed SiGe

1. Introduction

The hole mobility enhancement due to strain from various SiGe layer growth approaches has been widely adopted for aggressive CMOS technologies [1–3]. In addition to this advantage, the retarded diffusion of boron in SiGe is an extra benefit for device scaling. Boron diffusivity under this circumstance has been modeled in [7,8] with a diffusivity retardation that is an exponential function of the strain. Alternatively, it is claimed that the retardation is caused by Ge–B pairing instead [4,9]. A quantitative assessment of the respective contribution from mechanical strain and Ge doping is therefore necessary for accurate boron modeling inside and in the vicinity of SiGe. The boron extension and source/drain profiles in pMOSFET can be optimized with the resulting models. This paper will investigate boron diffusion in both strained and strain-relaxed SiGe including ultra-low energy, high concentration boron implant and spike RTA. The effects of implant damage, boron-interstitial cluster (BIC) model and transient enhanced diffusion (TED) effects will be also considered in the modeling procedure.

2. Experiments and results

There were two experiments performed using 300 mm, Czochralski-grown, ⟨1 0 0⟩ oriented, p-type silicon wafers with

* Corresponding author.

0921-5107/$ – see front matter © 2005 Elsevier B.V. All rights reserved.
doi:10.1016/j.mseb.2005.08.127

TSMC EXHIBIT 1034

Table 1
Brief descriptions for process flows and conditions

Experiment A (strain-relaxed SiGe)	Experiment B (strained SiGe)
2-μm SiGe film deposition 9%, 15%, 28%	Ge implant 1E15/cm^2, 1E16/cm^2 5 keV, 10 keV, 20 keV, 30 keV SiGe film formation by furnace 750 °C, RTA 900 °C or 980 °C
BF_2 implant 2 keV/1.3E15/cm^2 Spike RTA 970 °C, 1070 °C	BF_2 implant 2 keV/1.3E15/cm^2 Spike RTA 1050 °C

a starting resistivity of 5–100 Ω cm. One (experiment A) is a strain-relaxed SiGe experiment, and another (experiment B) is a strained SiGe experiment. A 2-μm thick strain-relaxed SiGe layer was deposited as described in [10], with various Ge concentrations, 9%, 15%, and 28% for experiment A (strain-relaxed SiGe). The Ge concentration was accurately extracted by secondary ion mass spectrometry (SIMS) in order to avoid the experimental variance when taking it from the setting of the film deposition system. Wafers in experiment B (strained SiGe) were implanted with Ge at a dose of 1×10^{15} cm^{-2} or 1×10^{16} cm^{-2} and at a variety of energies 5 keV, 10 keV, 20 keV, and 30 keV. Following the Ge implant, these wafers were annealed in an inert N2 ambient at a variety of temperatures either 750 °C furnace or 900 °C RTA or 980 °C RTA to form a strained SiGe layer. A BF2 implant followed with a dose of 1.3×10^{15} cm^{-2} and an energy of 2 keV for both experiments A and B. Finally, all wafers were annealed by a high temperature spike RTA that is widely used for ultra-shallow junction (USJ) formation. Table 1 shows the process flow and detailed conditions. Once the process was completed, both boron and Ge profiles were extracted with SIMS, using 750 eV O^{2+} primary ions with an oblique angle of incidence (45°) and 2×10^{-6} Torr oxygen-leak.

2.1. Result of experiment A (strain-relaxed SiGe)

Figs. 1 and 2 show the SIMS profiles for experiment A annealed at 970 °C and 1070 °C, respectively. The boron diffusion retardation is proportional to the Ge concentration. Fig. 3 shows the boron junction depth (Xj at 1×10^{18} cm^{-3}) at various

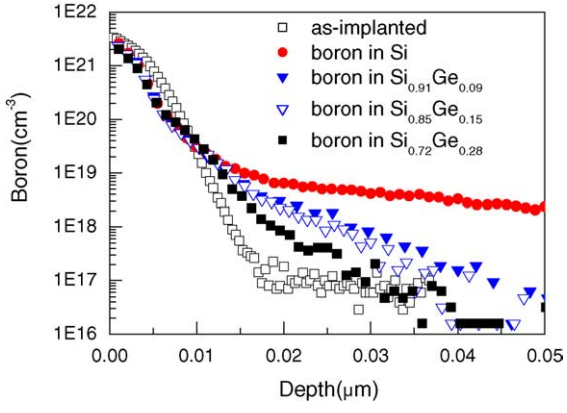


Fig. 1. Boron SIMS profiles of BF_2/2 keV/1.3×10^{15} cm^{-2} in experiment A (strain-relaxed SiGe) annealed at 970 °C.

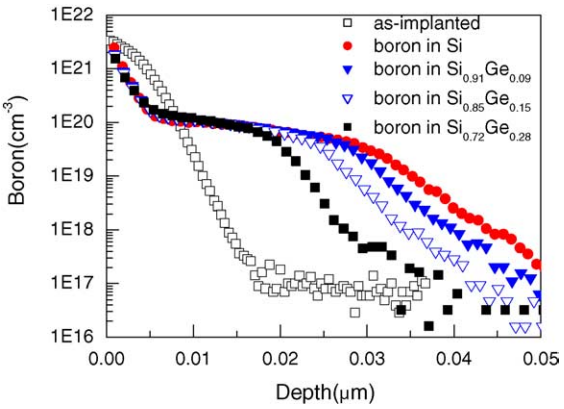


Fig. 2. Boron SIMS profiles of BF_2/2 keV/1.3×10^{15} cm^{-2} in experiment A (strain-relaxed SiGe) annealed at 1070 °C.

process conditions. The junction depth annealed at 970 °C (Xj at 970 °C) in silicon is relative deep. It was caused by significant tail diffusion resulting from TED, which occurs at low temperature. However, the Xj at 970 °C is always shallower than the Xj at 1070 °C in SiGe. The diffusivity retardation seems to be drastic at low temperature. At higher Ge concentration, a shallower junction depth is observed that implies certain interaction between boron and Ge, which impacts boron diffusivity.

2.2. Result of experiment B (strained SiGe)

Figs. 4 and 5 show the SIMS profiles of Ge and boron, respectively. Implant tables of boron and Ge were established by the SIMS profiles and fed into TSUPREM4 [11]. The shallowest (5 keV) Ge junction depth (Xj at 1×10^{18} cm^{-3}) is around 30 nm. It is deeper than the annealed boron profile, which makes sure that all boron dopant is impacted by the implanted Ge. Boron retarded diffusion was observed in Fig. 5, especially in the wafers processed with low Ge implant energy. We summarize the phenomena in Fig. 6 (Ge/1×10^{15} cm^{-2}) and Fig. 7 (Ge/1×10^{16} cm^{-2}). It is obvious that a lower Ge implant energy leads to shallower boron junction. We believe that the retarded diffusion is caused by both Ge concentration and stress. A shal-

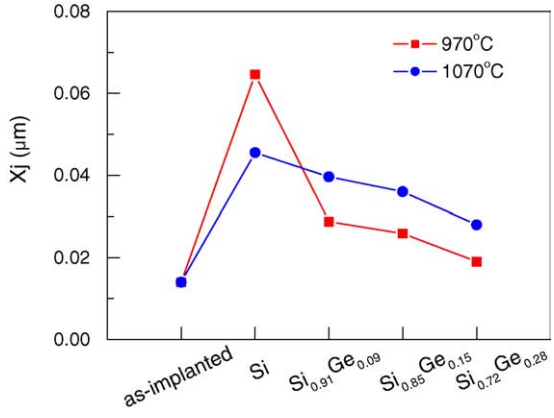


Fig. 3. Boron junction depth (at 1×10^{18}/cm^2) of BF_2/2 keV/1.3×10^{15} cm^{-2} in experiment A (strain-relaxed SiGe) annealed at 970 °C or 1070 °C in silicon, $Si_{0.91}Ge_{0.09}$, $Si_{0.85}Ge_{0.15}$, and $Si_{0.72}Ge_{0.28}$.

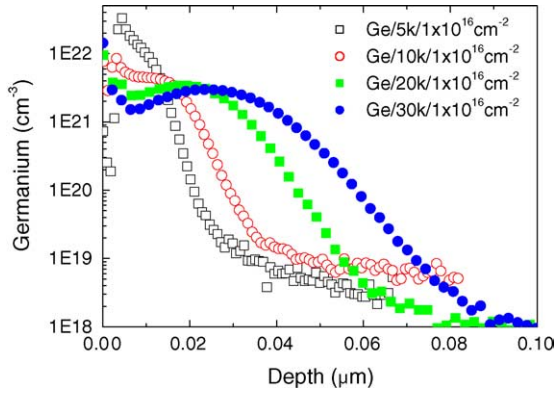


Fig. 4. Ge SIMS profiles in experiment B (strained SiGe) at a dose of 1×10^{16} cm^{-2} and at a variety of energies 5 keV, 10 keV, 20 keV, and 30 keV.

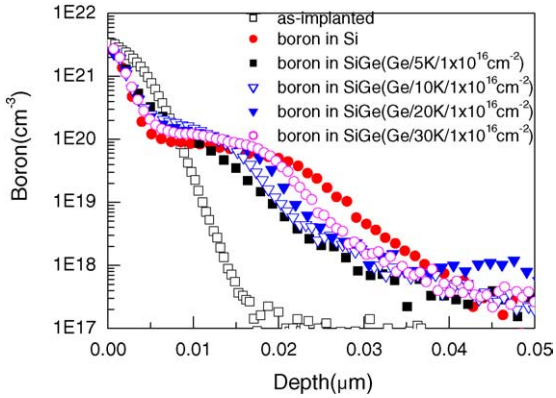


Fig. 5. Boron SIMS profiles of BF_2/2 keV/1.3 $\times$ 10^{15} cm^{-2}in experiment B (strained SiGe) annealed at 1050 °C.

lower profile and high concentration of Ge indeed gave more retardation. The SiGe formation temperature is another interesting topic in experiment B (strained SiGe). Figs. 6 and 7 also demonstrate that the final boron junction depth is almost independent on the formation temperature. We therefore adopted the wafers processed by 750 °C furnace for the SiGe formation and

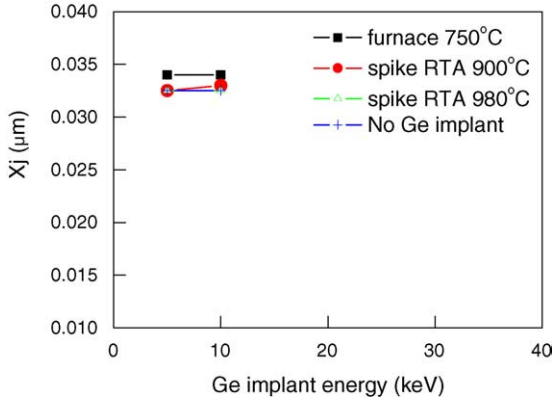


Fig. 6. Boron junction depth (Xj at 1×10^{18} cm^{-3}) vs. various Ge implant energy (5 keV and10 keV) with dosage 1×10^{15} cm^{-2}. There is no significant junction depth difference among the three methods (furnace 750 °C, spike RTA 900 °C, and spike RTA 980 °C) to form SiGe. Retarded diffusion is not observed in these three samples compared to the sample without Ge implant.

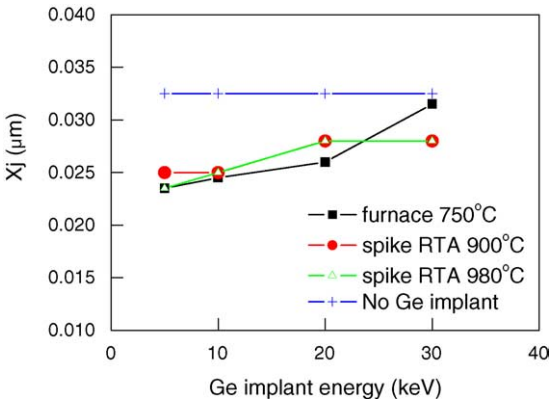


Fig. 7. Boron junction depth (Xj at 1×10^{18} cm^{-3}) vs. various Ge implant energy (5 keV, 10 keV, 20 keV, and 30 keV) with dosage 1×10^{16} cm^{-2}. There is no significant junction depth difference among the three methods (furnace 750 °C, spike RTA 900 °C, and spike RTA 980 °C) to form SiGe. Retarded diffusion is observed in these three samples compared to the sample without Ge implant.

1×10^{16} cm^{-2} Ge implant as the fitting target in the following modeling procedure.

3. Model calibration and discussion

Regarding boron diffusion behavior in strain-relaxed SiGe (experiment A), we can assume that it is related to Ge concentration effect only. Lever et al. [9] proposed that boron will be trapped by Ge and thus the diffusivity is therefore reduced. The ratio between mobile boron concentration and active boron concentration, the trapping ratio, was proposed to be an index to investigate this phenomenon. We tried to implement this model as well as fully coupled model into TSUPREM4, however, it is a big task because we have to write most of diffusion equations existing in TSUPREM4 with, USEIT [11], the feature of the TSUPREM4 modeling interface. It is caused by that the parameter "ni" in TSUPREM4 has two different meanings. One is the intrinsic concentration and another is a normalization factor. We cannot modify the intrinsic concentration in SiGe without changing the normalization factor. We therefore ignored the inaccuracy in intrinsic concentration but only implemented the trapping ratio into TSUPREM4 by USEIT. Figs. 8 and 9 show the results for experiment A (strain-relaxed SiGe) annealed at 970 °C and 1070 °C, respectively. Fig. 10 shows the trapping ratio versus Ge concentration at 970 °C and 1070 °C. A high Ge concentration and a low anneal temperature make more boron trapped by Ge and reduce the diffusion length. Therefore, we propose an empirical model that also describes the boron diffusion behavior under this circumstance well:

$$D_\mathrm{SiGe} = D_\mathrm{Si} \times \exp\left[-4.2\mathrm{E}-6 \times \exp\left(\frac{1.58}{kT}\right) \times \mathrm{Ge.Frac}\right] = D_\mathrm{Si} \times \exp(\Delta E_a) \quad (1)$$

where D_Si is the diffusivity of boron in silicon, T the anneal temperature (K) and Ge.Frac is germanium fraction. Because of the simplicity of this model, Fermi-level dependent diffusivity, fully coupled model and boron-interstitial cluster (BIC)

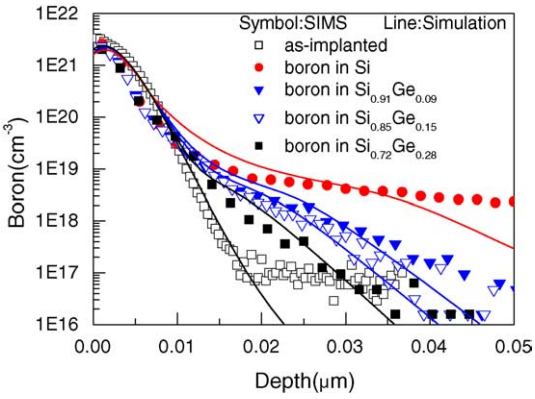


Fig. 8. The calibration result (lines) based on the trapping ratio model [9] and SIMS profiles (symbols) of BF_2/2 keV/1.3 × 10^{15} cm^{-2} in experiment A (strain-relaxed SiGe) annealed at 970 °C.

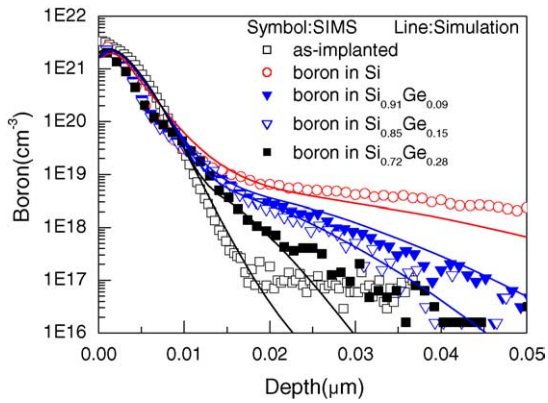


Fig. 11. The calibration result (lines) based on Eq. (1) and SIMS profiles (symbols) of BF_2/2 keV/1.3 × 10^{15} cm^{-2} in experiment A (strain-relaxed SiGe) annealed at 970 °C.

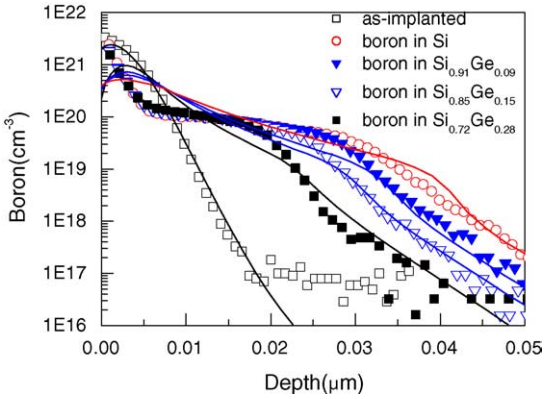


Fig. 9. The calibration result (lines) based on the trapping ratio model [9] and SIMS profiles (symbols) of BF_2/2 keV/1.3 × 10^{15} cm^{-2} in experiment A (strain-relaxed SiGe) annealed at 1070 °C.

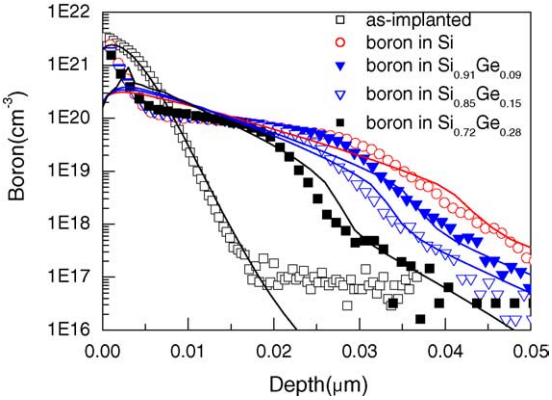


Fig. 12. The calibration result (lines) based on Eq. (1) and SIMS profiles (symbols) of BF_2/2 keV/1.3 × 10^{15} cm^{-2} in experiment A (strain-relaxed SiGe) annealed at 1070 °C.

model are easily to couple together to simulate boron diffusion in TSUPREM4. Contrary to the simple models for the low boron concentrations used in [4,5], these models are necessary to model experiments A and B. Based on this model, the boron diffusivity in strain-relaxed SiGe is therefore well modeled at various anneal temperatures (Figs. 11 and 12).

The retarded diffusivity versus Ge concentration extracted from this model and the trapping ratio versus Ge concentration extracted based on Lever's concept are also shown in Fig. 13. It is obvious that these two parameters are quite close to each other. Regarding the calibration of strained SiGe (experiment B), Cowern et al. [7] proposed a model to describe the relationship between mechanical strain and boron diffusivity. However, the

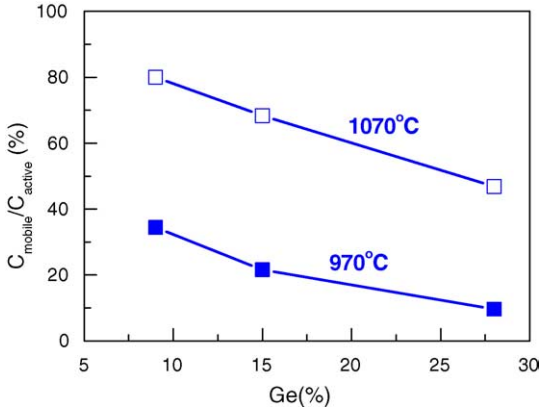


Fig. 10. The trapping ratio of boron extracted from Figs. 8 and 9 based on the trapping ratio model [9].

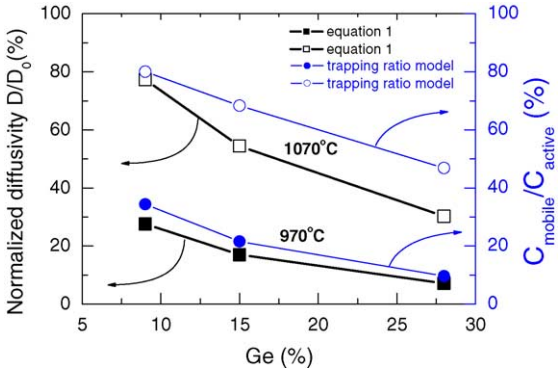


Fig. 13. Both the retarded diffusivity extracted from Eq. (1) and the trapping ratio extracted from the trapping ratio model [9]. Although different methods are used, the values of these two extracted parameters are close to each other.

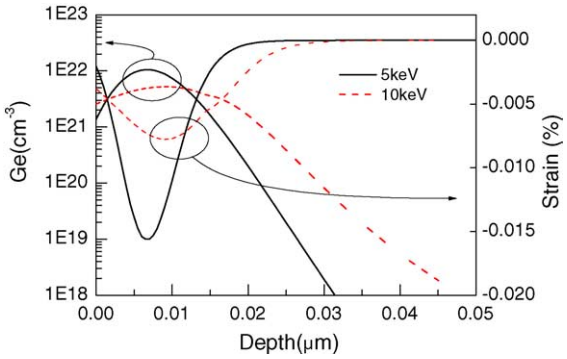


Fig. 14. The Ge profiles and Ge.Strain used in Eq. (2).

Ge–B pairing effect was ignored in his model. A new model to include both Ge–boron pairing and strain effects is necessary to model experiment B (strained SiGe). The new model is proposed below:

$$D_\mathrm{SiGe} = D_\mathrm{Si} \times \exp\left(\mathrm{Ge.strain} \times \left(\frac{Q'_{\mathrm{B}(i)}}{kT}\right)\right) = D_\mathrm{Si} \times \exp(\Delta E_\mathrm{b}) \quad (2)$$

where Ge.strain is the strain caused by lattice mismatch between Ge and silicon $Q'_{\mathrm{B}(i)} = -6.8\,\mathrm{eV/unit\ strain}$.

Fig. 14 shows the Ge concentration and Ge.strain for the condition of Ge/5 keV/$1 \times 10^{16}\,\mathrm{cm}^{-2}$ and Ge/10 keV/$1 \times 10^{16}\,\mathrm{cm}^{-2}$. The absolute value of Ge.strain is proportional to Ge concentration such as the relationship described in Eq. (2). The combined effect of both the Ge concentration effect (ΔE_a) and the strain dependence effect (ΔE_b) on boron diffusivity in SiGe can be expressed as:

$$D_\mathrm{SiGe} = D_\mathrm{Si} \times \exp(\Delta E_\mathrm{a} + \Delta E_\mathrm{b}) \quad (3)$$

Fig. 15 shows the calibration result of experiment B (strained SiGe) based on Eq. (3). The strain dependent change in the activation energy, $Q'_{\mathrm{B}(i)}$ in [3], was extracted as 0.068 eV/percent-strain, instead of 0.17 eV/percent-strain found in [3]. Fig. 16 shows the detailed diffusivity retardation component under both mechanical strain and Ge doping. Both contribute a similar

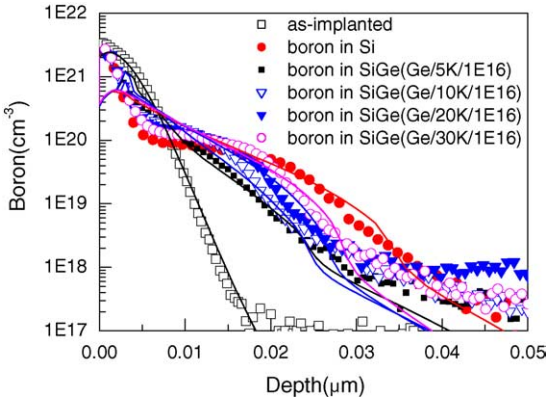


Fig. 15. The calibration result (lines) based on Eqs. (1) and (2) and SIMS profiles (symbols) of BF_2/2 keV/$1.3 \times 10^{15}\,\mathrm{cm}^{-2}$ in experiment B (strained SiGe) annealed at 1050 °C.

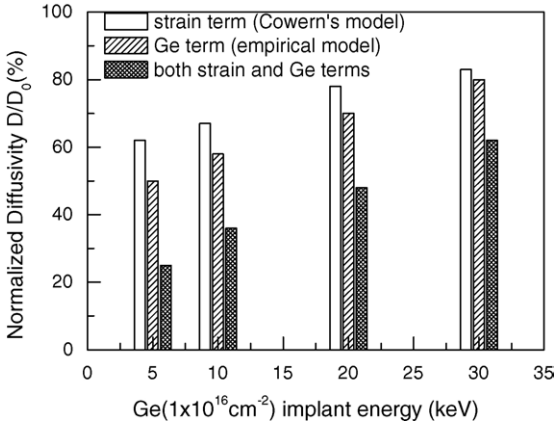


Fig. 16. The bar chart to show respective retardation contributions from various models at experiment B (strained SiGe).

amount to the retardation, Ge term retards slightly more. The importance of the retardation contribution from mechanical strain is therefore revealed and cannot be ignored in strained SiGe. It is quite important to model the boron profile in the gate ledge of a pMOSFET [2,3] because only strain but Ge exists there.

4. Conclusion

We have calibrated USJ boron retarded diffusion in both strain-relaxed and strained SiGe based on experiments. The retardation components from Ge doping and mechanical strain are identified separately. Empirical equations are used to model the dependence on Ge concentration and mechanical strain, respectively. The fully coupled model and the boron-interstitial cluster (BIC) model are necessary for the simulation of aggressively scaled devices; these effects are easily linked together with our models to simulate boron diffusion. Based on the calibration result, we conclude that both mechanical strain and Ge concentration dependent retardation significantly impact boron diffusion behavior in strained SiGe.

References

[1] M. Shima, T. Ueno, T. Kumise, H. Shido, Y. Sakuma, S. Nakamura, Symposium on VLSI Technology Technical Digest, 2002, pp. 94–95.
[2] T. Ghani, M. Armstrong, C. Auth, M. Bost, P. Charvat, G. Glass, T. Hoffmann, K. Johnson, C. Kenyon, J. Klaus, B. McIntyre, K. Mistry, A. Murthy, J. Sandford, M. Silberstein, S. Sivakumar, P. Smith, K. Zawadzki, S. Thompson, M. Bohr, International Electron Devices Meeting Technical Digest, December 2003, pp. 978–980.
[3] P. Bai, C. Auth, S. Balakrishnan, M. Bost, R. Brain, V. Chikarmane, R. Heussner, M. Hussein, J. Hwang, D. Ingerly, R. James, J. Jeong, C. Kenyon, E. Lee, S. Lee, N. Lindert, M. Liu, Z. Ma, T. Marieb, A. Murthy, R. Nagisetty, S. Natarajan, J. Neirynck, A. Ott, C. Parker, J. Sebastian, R. Shaheed, S. Sivakumar, J. Steigerwald, S. Tyagi, C. Weber, B. Woolery, A. Yeoh, K. Zhang, M. Bohr, International Electron Devices Meeting Technical Digest, December 2004, pp. 657–660.
[4] P. Kuo, J.L. Hoyt, J.F. Gibbons, J.E. Turner, D. Lefforge, Appl. Phys. Lett. 66 (January (5)) (1995) 580–582.

[5] N.R. Zangenberg, J. Fage-Pedersen, J. Lundsgaard Hansen, A. Nylandsted Larsen, J. Appl. Phys. 94 (September (6)) (2003) 3883–3890.
[7] N.E.B. Cowern, P.C. Zalm, P. van der Sluis, D.J. Gravesteijn, W.B. de Boer, Phys. Rev. Lett. 72 (April (16)) (1994) 2585–2588.
[8] C.-L. Liu, M. Orlowski, A. Thean, A. Barr, T. White, B.-Y. Nguyen, H. Rueda, X.-Y. Liu, Materials Research Society Symposium Proceedings, vol. 765, 2003, p. D5.9.1.
[9] R.F. Lever, J.M. Bonar, A.F.W. Willoughby, J. Appl. Phys. 83 (February (4)) (1998) 1988–1994.
[10] C.-C. Lin, C.-H. Wang, C.-H. Ge, C.-C. Huang, T.-C. Chang, L.-G. Yao, S.-C. Chen, M.-S. Liang, F.-L. Yang, Y.-C. Yeo, C. Hu, International Conference on Solid State Devices and Materials, 2002, pp. 12–13.
[11] TSUPREM-4, Version 2003.06, Synopsys.