Modeling Dopant Diffusion in Strained and Strain-Relaxed Epi-SiGe

Yi-Ming Sheu[1], Tsung-Yi Huang[1], Yu-Ping. Hu[1], Chih-Chiang Wang[1], Sally Liu[1], Ray Duffy[2], Anco Heringa[2], Fred Roozeboom[3], Nick E.B. Cowern[4], and Peter B. Griffin[5]

[1]TCAD project, Device Engineering Division, R&D, Taiwan Semiconductor Manufacturing Company, No.9, Creation Rd. 1, Science-Based Industrial Park, Hsin-Chu, Taiwan, 300-77, R.O.C. (ymsheu@tsmc.com)
[2]Philips Research Leuven, Kapeldreef 75, 3001 Leuven, Belgium
[3]Philips Research Laboratories Eindhoven, Prof. Holstlaan 4, 5656 AA Eindhoven, The Netherlands
[4]Advanced Technology Institute, University of Surrey, Guildford, Surrey GU2 7XH, UK
[5]Center for Integrated Systems, Stanford University, Stanford, CA, 94305-4070, USA

Abstract – **Ultra-shallow arsenic and boron diffusion in both strained and strain-relaxed SiGe has been investigated in this paper. Significant arsenic diffusion enhancement and boron diffusion retardation have been observed. Strained SiGe was found to have a stronger arsenic diffusion enhancement. Empirical equations in Arrhenius form have been created and incorporated into numerical simulation to successfully model the diffusion dopant profiles.**

I. INTRODUCTION

The utilization of SiGe in the semiconductor industry has been extended from heterojunction bipolar transistor to CMOS technology to achieve an aggressive performance goal as the technology marches toward the nanometer regime [1]-[3]. The study of high concentration and ultra-shallow dopant diffusion in SiGe is of great importance for modern technology development. Both mechanical strain and germanium pairing effects play important roles in dopant diffusion in the SiGe epi-layers. Boron diffusion has been reported to be retarded by both the existence of germanium and biaxial compressive mechanical strain in the SiGe epi-layer [4, 5]. Arsenic diffusion enhancement in the SiGe epi-layer has been reported, but the germanium pairing and mechanical strain effects were not decoupled [6].

In this paper, an experiment into low energy and high dosage ion implantation, and short-annealing-time dopant diffusion of arsenic and boron in both strained and strain-relaxed SiGe was conducted to investigate ultra-shallow junction diffusion in SiGe at various temperatures. Diffusion models based on the Arrhenius form explaining both the mechanical strain and the germanium pairing effects have been proposed and incorporated into the numerical simulation to model the diffusion profiles.

II. EXPERIMENT

In the experiment, SiGe epi-layers of two concentration levels, 20% and 30%, and two layer thicknesses, 50nm and 4μm were grown on silicon wafers. The 4μm SiGe layers were grown starting from 2μm graded germanium concentration, increasing from 0 to the target concentration and then another 2μm constant target germanium concentration level, which is presumed to be strain-relaxed. The 50nm SiGe epi-layer was grown starting with the target germanium concentration level, which is presumed to be strained. Pure silicon wafers were used for comparison. BF_2 and arsenic with energy of 2keV and a dosage of $1\times10^{15}cm^{-2}$ were implanted into two independent wafer sets. Finally, the wafers were annealed at three different temperatures, 900°C, 1000°C, and 1025°C, using the spike RTA. After the wafer process was completed, the dopant profiles were analyzed using secondary ion mass spectrometry (SIMS). The SIMS analysis conditions were 750eV O_2+ primary ion for the boron profiles and 500eV Cs+ primary ion for the arsenic and germanium profiles.

III. MODEL CALIBRATION AND DISCUSSION

The germanium concentration levels as extracted from SIMS, are listed in Table 1. Figures 1 and 2 show the SIMS profiles for arsenic and boron, respectively, at annealing temperatures of 900C^o, 1000°C and 1025°C. The general concept for simulating the diffusion in SiGe is to express the influence of germanium on the dopant diffusivity in an Arrhenius form [7]. From the SIMS dopant profiles, it was observed that the activation energy term in the Arrhenius equations for both the germanium pairing and the strain effect must be temperature-dependent. Thus, three equations were proposed to account for the dopant diffusion in SiGe,

$$D_SiGe(Ge) = D_Si \times \exp[\mathrm{A} \times \exp(\mathrm{B}/T) \times Ge.Frac] = D_Si \times \exp(\Delta E_a) \quad (1)$$

$$D_SiGe(strain) = D_Si \times \exp[(Ge.strain \times (\exp(\mathrm{C}/T) \times \mathrm{D})/kT] = D_Si \times \exp(\Delta E_b) \quad (2)$$

$$D_SiGe(Ge, strain) = D_Si \times \exp[(\Delta E_a + \Delta E_b)] \quad (3)$$

where
D_Si is the dopant diffusivity in silicon, *T* is the anneal temperature (K), *Ge.Frac* is the germanium mole fraction, *Ge.strain* is the strain in the SiGe layers. A, B, C and D are coefficients depending on dopant impurities.

A numerical process simulator, TSUPREM4, was used to perform the dopant profile simulation. Equations (1)-(3) were incorporated into the simulator through the user-specified equation interface to adaptively calculate dopant diffusivity during the process simulation. In contrast to the low dopant concentrations used in [4, 8], it is first necessary to calibrate the Fermi-level dependent diffusivity, fully-coupled model and dopant cluster model using dopant profiles in pure silicon samples. Then the dopant diffusivity in strain-relaxed SiGe is well-modeled at various annealing temperatures (Figures 1 and 2) using equation (1). Finally, equations (2) and (3) were used to model dopant profiles in strained SiGe. The mechanical strain was calculated from the Vegard's law. Table 2 shows the extracted values of coefficients A, B, C, and D for arsenic and boron in this experiment. The coefficient C of boron is zero, which means there is the strain dependent activation energy is independent of temperature. On the other hand, C and D of arsenic diffusion shows strong temperature dependency of strain activation energy. The boron resultant coefficients are close to previous work [5]. Fig. 3 shows the diffusivity ratios under both mechanical strain and germanium doping effect versus germanium concentration for the various temperatures. The strain effect on the arsenic diffusion enhancement significantly increases as the temperature increases.

IV. CONCLUSION

High concentration ultra-shallow arsenic and boron diffusion in both strained and strain-relaxed SiGe epi-layers has been investigated. Based on the experiment results, it can be concluded that both the mechanical strain and the germanium concentration enhance arsenic diffusion and retard boron diffusion in the strained SiGe epi-layer. The diffusion components from the germanium doping and mechanical strain effect are decoupled and also identified as being temperature-dependent. Diffusion models explaining both the mechanical strain and the germanium pairing effects have been proposed, and the experimental dopant profiles have been successfully modeled. A simple empirical equation satisfactorily fits the diffusion dependence on the germanium concentration and mechanical strain for both arsenic and boron.

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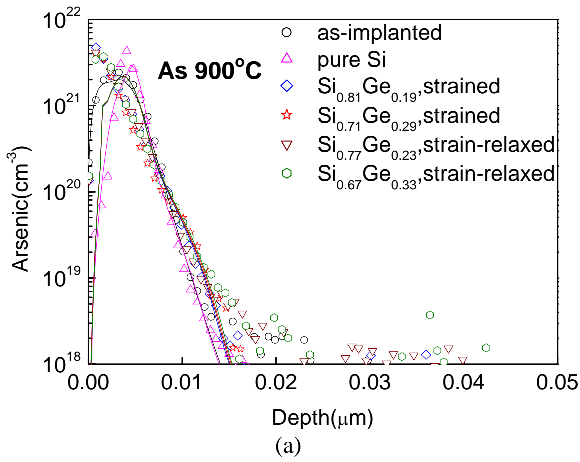
TABLE 1
Extracted germanium concentration from the SIMS

	Ge concentration
Strained 50nm SiGe A	19%
Strained 50nm SiGe B	29%
Strain-relaxed 2μm SiGe A	23%
Strain-relaxed 2μm SiGe B	33%

TABLE 2
Extracted A, B, C, and D in the equations from dopant profile modeling

	As	B
A (1/mole fraction)	$7.93\text{x}10^{3}$	$-4.2\text{x}10^{-6}$
B (K)	$-8.65\text{x}10^{3}$	$1.83\text{x}10^{4}$
C (K)	$-3.14\text{x}10^{4}$	0
D (eV/percent strain)	$2.4\text{x}10^{11}$	-6.8



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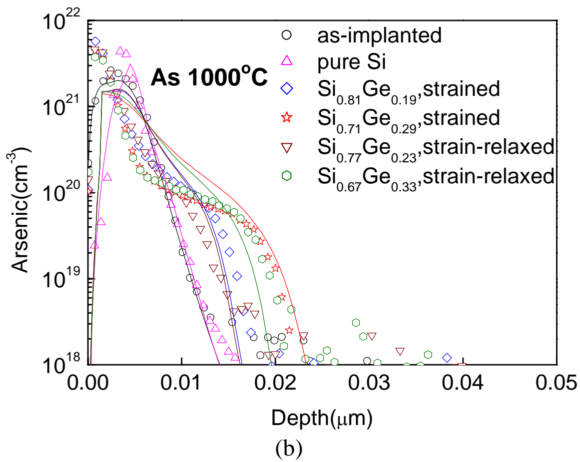

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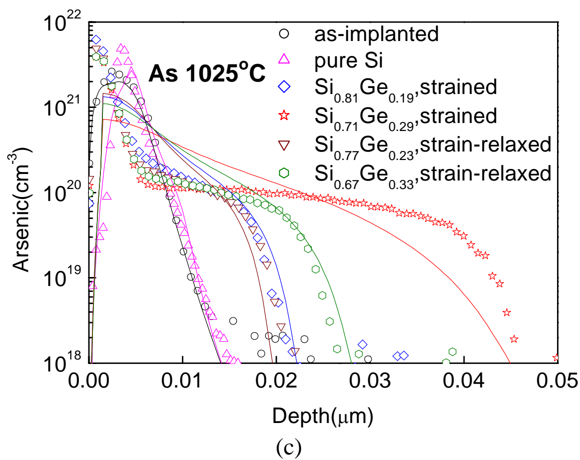
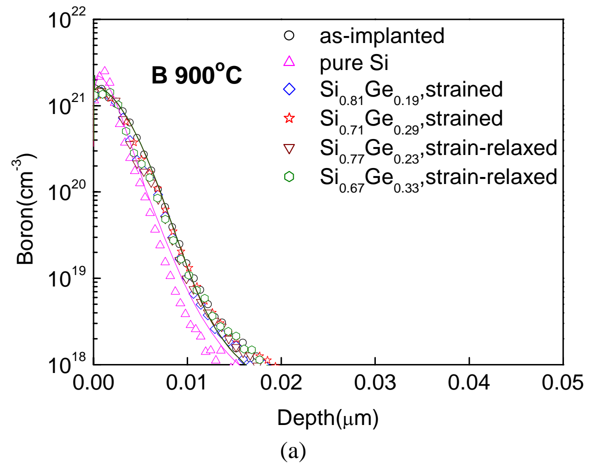
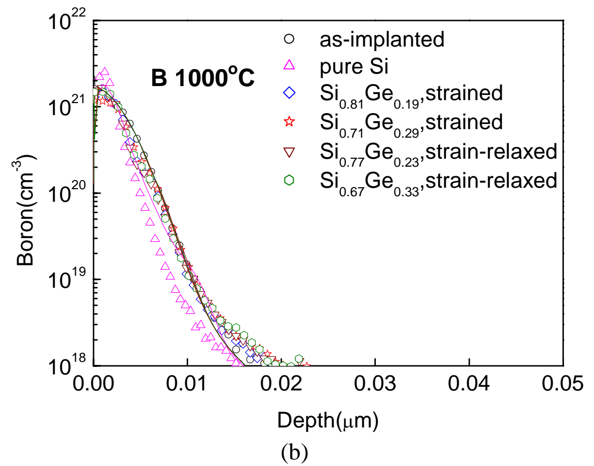


(c)

Figure 1 Arsenic dopant profiles in silicon and different SiGe layers after (a) 900°C, (b) 1000°C, and (c) 1025°C RTA. Symbols indicate the SIMS data and the solid lines are the simulation results.



(a)



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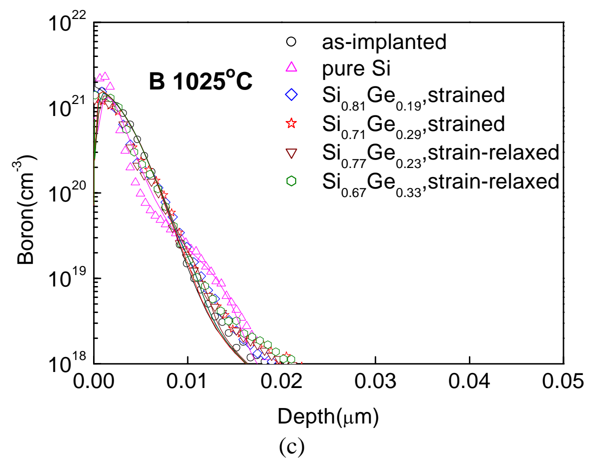
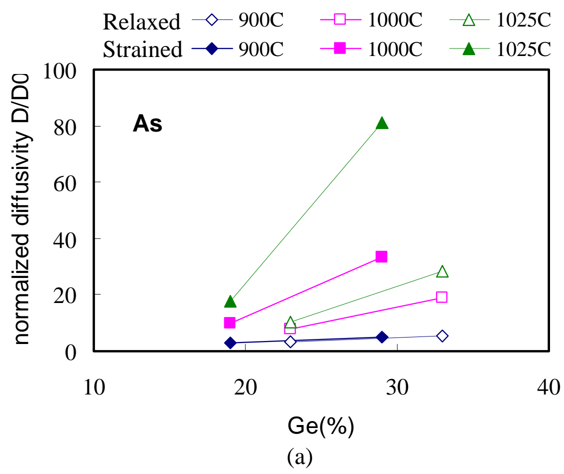


(c)

Figure 2 Boron dopant profiles in silicon and different SiGe layers after (a) 900°C, (b) 1000°C, and (c) 1025°C RTA. Symbols indicate the SIMS data and the solid lines are the simulation results.



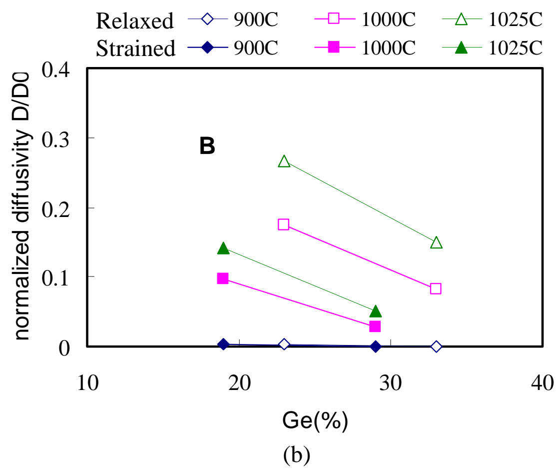


Figure 3 Normalized diffusivities versus germanium concentration for (a) arsenic and (b) boron.