Modeling of the Diffusion of Implanted Boron in Strained $Si/Si_{1-x}Ge_x$

Huilong Zhu*, Kam-leung Lee**, O. Dokumaci*,
P. Ronsheim*, F. Cardone**, S. Hegde**, U. Mantz*, P. Saunders**
IBM Semiconductor Research and Development Center (SRDC)
*Microelectronics Division, Hopewell Junction, NY 12533
**IBM T.J. Watson Research Center, Yorktown Heights, NY 10598
E-mail: huilong@us.ibm.com

***Abstract* - The diffusion of implanted boron in strained $Si/Si_{1-x}Ge_x$ was investigated. A continuum segregation model (CSM) is presented to describe the phenomenon of B pile-up into the germanium profile. An analytic formula is obtained for Ge pre-amorphization and a modified pre-amorphization model is used in TSUPREM4 in order to accurately model our measurement data. Our simulations of boron diffusion are in reasonable agreement with our SIMS data. Comparison of the CSM with the model of immobile boron-germanium clusters is also discussed.**

I. INTRODUCTION

Modeling of dopant diffusion in strained $Si/Si_{1-x}Ge_x$ ($SSi/Si_{1-x}Ge_x$) becomes increasingly important since $SSi/Si_{1-x}Ge_x$ is a candidate for strained Si CMOS (SSi-CMOS) devices [1] and since the diffusion of dopant in SiGe can form parasitic barriers at the heterojunction in a heterojunction bipolar transistor (HBT). In these devices, even dopant diffusion of a few nanometers can be significant. Therefore, in order to efficiently design and develop SSi-CMOS and HBT devices, it is crucial to understand and accurately model the diffusion behavior of dopant in $SSi/Si_{1-x}Ge_x$ as a function of chemical composition, anneal temperature and time. However, the existence of stress and Ge in $SSi/Si_{1-x}Ge_x$ complicates the modeling of dopant diffusion, since the stress and Ge affect the band-gap and the formation energy of defects.

In this paper, we model the diffusion of implanted boron in $SSi/Si_{1-x}Ge_x$ based on published models and our new segregation model. We also present an analytical formula and a modified model for Ge pre-amorphization. The formula and the modified model were calibrated to our experimental data. USEIT [2] was used to implement the models into TSUPREM4. Boron SIMS data were used to verify and calibrate our simulation results.

II. BORON DIFFUSION EXPERIMENTS

Before describing our model, we discuss our experimental data. Figure 1 shows B SIMS profiles in a $SSi/Si_{0.8}Ge_{0.2}$ bilayer structure after RTA at 1000C for 5 seconds. The $SSi/Si_{0.8}Ge_{0.2}$ layers were created using a UHCVD process. X-ray analysis showed that the $Si_{0.8}Ge_{0.2}$ substrate is ~98% relaxed. Before the RTA, the $SSi/Si_{0.8}Ge_{0.2}$ was pre-amorphized by Ge implantation and followed by B implantation with a given energy at either of two different doses. The Si/SiGe interface locates around the normalized depth of 1.0. It can be seen that there is a peak in B concentration near the Si/SiGe interface. This indicates that B prefers to stay in or segregates into SiGe. A similar phenomenon was first observed by Hu et al [3]. Hu treated Si and $Si_{1-x}Ge_x$ as two different phases and

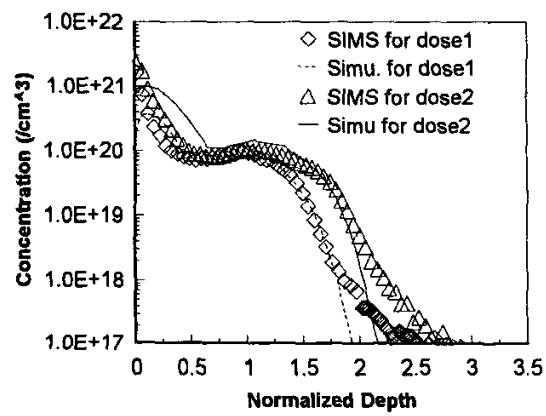

Figure 1 Boron diffusion in $SSi/Si_{0.8}Ge_{0.2}$. The interface of Si/SiGe is around the normalized depth of 1.0. One can see that B segregates into SiGe side after 1000C 5 seconds RTA.

pointed out that the B segregation coefficient between Si and $Si_{1-x}Ge_x$ is about 1.35 for x=0.1.

III. CONTINUUM SEGREGATION MODEL

It is well known that Ge diffuses during high temperature annealing and the boundary between Si and SiGe is no longer sharp. In this case, we need a "*continuum segregation*" model to consider the B segregation effect in Si/SiGe structures. To do so, we first

need to get an expression for the boron potential energy in $Si_{1-x}Ge_x$ as a function of x. This is because B segregation occurring between the two materials is caused by the difference of B potential energies in the materials. Since the two elements, Si and Ge, are fully miscible, we assume that SiGe is chemically disordered. Therefore, as shown in

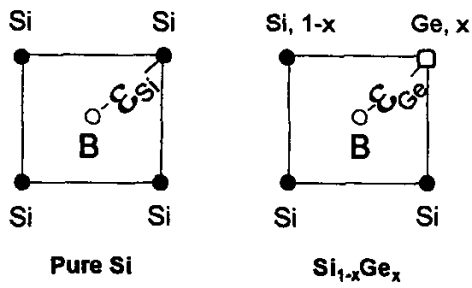

Figure 2 Schematic of a substitutional boron in pure Si and $Si_{1-x}Ge_x$ crystals. Solid circle, opened circle, and opened square represent Si, boron, and Ge atoms, respectively.

Fig. 2, we can write the potential energy of a boron atom in $Si_{1-x}Ge_x$ as

$$E_B(x) = \sum_i (1-x)\varepsilon_{Si}(i) + \sum_i x\varepsilon_{Ge}(i) = E_{Si} + x\Delta E_{Si\text{-}Ge}, \quad (1)$$

where E_{Si} and $\Delta E_{Si\text{-}Ge}$ are B energy in pure Si and the difference of B energies in pure Si and pure Ge, respectively. The value of $\Delta E_{Si\text{-}Ge}$ is used to fit experimental data. The parameter of ε_{Si} is the pair interaction between the boron atom and a Si atom. The sum is over all neighbors of the boron atom. The definition of ε_{Ge} is similar to ε_{Si}.

Equation 1 gives the relationship between boron energy and Ge composition in $Si_{1-x}Ge_x$. The gradient of the B energy can cause B diffusion or yield an additional drift term in the B diffusion equation:

$$\frac{\partial C_B}{\partial t} = \nabla \bullet (\nabla(D_B C_B C_I / C_I^\star) + q\frac{D_B C_B C_I}{kTC_I^\star}\vec{E} + \Delta E_{Si\text{-}Ge}\frac{D_B C_B C_I}{kTC_I^\star}\nabla(C_{Ge}/C_0)), \quad (2)$$

where C_B, C_{Ge}, and C_0 are boron concentration, germanium concentration, and lattice density of Si, respectively. C_I and C_I^* are non-equilibrium and equilibrium interstitial concentrations. The vector of $\vec{E}$ is electrical field, q is electron charge, k is the Boltzmann constant and T is absolute temperature. The third term on the right-hand side of Eq. 2 is the drift term owing to the gradient of Ge concentration.

We implemented Eq. 2 into TSUPREM4 using USEIT. In addition, the activation and interface trap models in TSUPREM4 were used and calibrated to consider the dose effect on B diffusion. The value of Ge diffusivity used in our simulations is close to that obtained by Zangenberg *et al* [6].

IV. BORON DIFFUSIVITY IN $Si_{1-x}Ge_x$

It was found that boron diffusivity depends exponentially on strain and Ge composition in SiGe [4, 5]. To describe stress and Ge composition effects on B diffusion in $SSi/Si_{1-x}Ge_x$, we combine the formulae of B diffusivity given by Moriya *et al* [4] and Cowern *et al* [5] and express B equilibrium diffusivity as

$$D_B=[D_0+D_p p/n_i \exp(-(Q_{ps}+Q_{pc})x/kT)]\exp(-(Q_s+Q_c)x/kT), \quad (3)$$

where Q_s and Q_c are coefficients for stress and composition effects on formation energy of interstitials. Q_{ps} and Q_{pc} are reflect the band-gap narrowing effect. The p and n_i are the hole and intrinsic carrier concentrations, respectively.

For our simulations, the Ge mole fraction is less than 0.3. In this case, B diffusion is predominantly via an interstitial mechanism [7]. Therefore, the TED effect on B diffusion is taken into account by multiplying the B diffusivity (given by Eq. (3)) by C_I/C_I^*.

V. Ge PRE-AMORPHIZATION

To calculate Ge pre-amorphization thickness as a function of implant dose and energy, we measured the amorphous layer thickness using ellipsometry and fitted the thickness by the following analytic formula

$$T_{amorp} = \alpha d^\beta E^\gamma, \quad d > d_c \quad (4)$$

where T_{amorp} denotes the amorphous thickness. E, d, and d_c represent Ge implant energy, dose, and amorphization threshold. The parameters α, β, and γ are determined by the experimental data. Merely using the amorphization model in TSUPREM-4, we could not match our experimental data even after calibration. We found that the scale factor (see Ref. 2), S_{FP}, of Frenkel-pairs depends on Ge implant energy:

$$S_{FP} = \zeta - \ln(E/\xi), \quad 100\text{ keV} > E > 5\text{ keV}, \quad (5)$$

where ζ and ξ are constants and E is Ge implant energy. The formation of amorphous Si is determined by the concentration of Frenkel-pairs/interstitials generated by Ge implantation and an amorphous threshold. Since the

number of Frenkel-pairs in TSUPREM4 is calculated by the model of Hobler and Selberherr (HS) [8], either the HS model or the amorphous threshold may need to be modified, especially for low energy Ge implants.

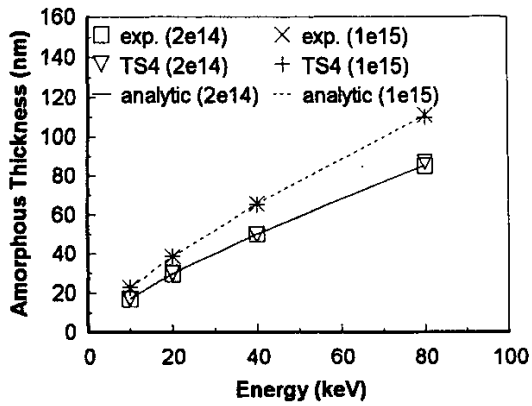

Figure 3 Ge pre-amorphization thickness versus Ge implant energies at doses $2x10^{14}cm^2$ and $1x10^{15}cm^2$. Both the analytic formula and calibrated TS4 results are excellently in agreement with experimental ellipsometry data.

Figure 3 shows the amorphous thickness as a function of dose and energy of Ge implants from our experiments, as well as the results of the analytic formula and the calibrated amorphization model using Eq. 5. Both the analytic formula and the calibrated amorphization model match the experimental data very well.

To date, no research has been done to study the Ge composition effect on Ge pre-amorphization in SiGe. As an approximation, we applied the Ge pre-amorphization model in Si to the SSi/SiGe structure. It is a reasonable approximation since in our case most amorphization takes place in the strained Si cap.

VI. SIMULATION RESULTS

With our new model, simulation results can match B SIMS in a range of doses, implant energies, annealing temperatures, and Ge compositions. We show a few examples of them in Figs. 1 and 4. We find that our simulation of B concentration for dose2 (high dose) in Fig. 1 is much higher than the SIMS near the surface. This indicates that the activation and/or interface trap models in TSUPREM-4 may need to be modified for high dose B diffusion. We believe that the mismatch in the diffusion tails in Fig. 1 is because the tail parts of the as-implanted profiles were not simulated accurately enough by TSUPREM4. Actually, in Fig. 4 the simulations started with as-implanted SIMS profiles and the tail parts of the simulated diffusion profiles fitted the corresponding SIMS profiles quite well. In the simulations, we assume that the stress in the Si cap remains after amorphous layer recrystallization. Although no detailed research has been done to study how regrowth changes the stress in the Si cap, it has been seen that RTA processes did not cause a significant relaxation of the stress in the Si cap [9].

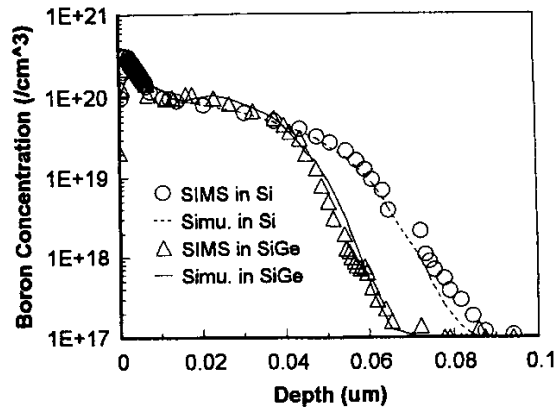

Figure 4 Boron diffusion profiles after RTA at 1000C for 5 seconds in pure Si and $SSi/Si_{0.8}Ge_{0.2}$. Our simulation results show that the B diffusivity dependence on Ge composition given by Eq. 2 is accurate enough to describe our SIMS data.

To compare the B segregation effect with SIMS, we plotted our simulation results with and without the segregation model against the SIMS data in Fig. 5. One

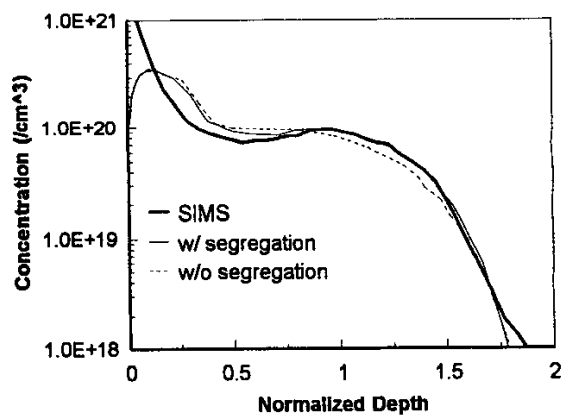

Figure 5 Comparison of simulated results w/ and w/o the segregation model with the SIMS in $SSi/Si_{0.8}Ge_{0.2}$ after RTA at 1000C for 5 s. Thick solid line represents the SIMS. With the segregation model, the simulation plotted by thin solid line shows a peak around the Normalized Depth = 1.0 at which the interface of Si and SiGe locates.

can see that without the B segregation model, the B profile monotonically decreases with increasing depth around the Si/SiGe interface near the normalized depth of 1. Since the diffusivity of boron in SiGe is smaller than that in the Si cap, it makes the part of the simulated profile around the Si/SiGe interface flatter than that in pure Si (see the dotted line in Fig. 4). However, there is no peak near the normalized depth of 1. The SIMS data show a peak around the Si/SiGe interface which can be explained by the B segregation model.

The model of boron-germanium clusters (BGeC) can predict boron pile-up in thin SiGe layers of HBT structures [10]. In the model of BGeC, the boron is assumed to be immobile, but electrically active. This means that BGeC can affect B diffusion through their electrical field and Fermi level effect (change of p/n_i), although the boron in the BGeC can not diffuse. In comparing the BGeC model with our segregation model, we expect that the segregation model gives larger diffusion

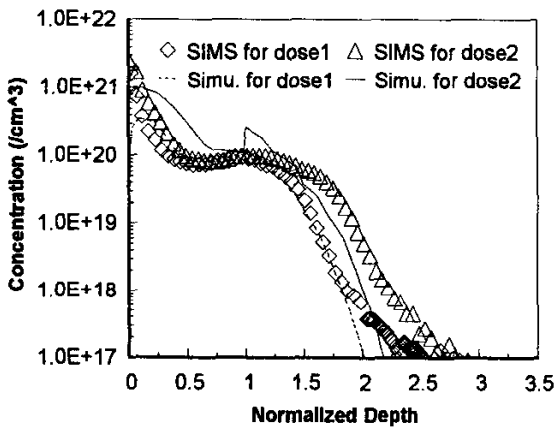

Figure 6 Comparison of BGeC model with SIMS data. For high dose (dose2), BGeC model gives a less diffusion than the SIMS.

than does the BGeC model. This is due to boron atoms in SiGe being treated as mobile as well as electrically active in the segregation model. We simulated the SIMS data shown in Fig. 1 using the BGeC model and plotted the simulated results in Fig. 6. In this simulation, similar to the calibration of the segregation model, we calibrated the BGeC model to the SIMS for the low dose case (dose1) and applied the calibrated parameters to the dose2 case. Comparing Figs. 1 and 6, one can see that the segregation model gives a better match for the dose2 case than does the BGeC model. The BGeC model predicts less boron diffusion and a higher segregation peak than is seen in the SIMS.

VII. SUMMARY

Implanted boron diffusion in strained Si/SiGe was investigated. We presented a segregation model to describe the phenomenon of B pile-up within the germanium profile. Comparing with a boron-germanium cluster model, our segregation model gave a better fit to the SIMS data. We also obtained an analytic formula for Ge pre-amorphization and modified the TSUPREM4 pre-amorphization model in order to accurately fit our measurement data of Ge pre-amorphization. Our simulations of boron diffusion are reasonably in agreement with our SIMS data.

ACKNOWLEDGMENT

The author, HZ, thanks C. Murthy, P. Oldiges, Z. Ren, R. Young, and R.J. Miller for interesting discussions.

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