Comparison of arsenic diffusion in $Si_{1-x}Ge_x$ formed by epitaxy and Ge^+ implantation

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A comparison is made of arsenic diffusion in $Si_{0.95}Ge_{0.05}$ produced by epitaxy and ion beam synthesis using a 2×10^{16} cm^{-2} Ge^+ implant into silicon. The arsenic diffusion depth at 1025 °C in the $Si_{0.95}Ge_{0.05}$ epitaxy sample is enhanced by a factor of 1.26 compared with a similar Si control sample and by a factor of 1.30 in the ion beam synthesized sample. The arsenic diffusion in the $Si_{0.95}Ge_{0.05}$ epitaxy sample is modeled by increasing the arsenic diffusion coefficient from the Si value of 1.92×10^{-15} to 5.15×10^{-15} cm^2 s^{-1}, and in the ion beam synthesized sample by using the same diffusion coefficient of 5.15×10^{-15} cm^2 s^{-1} and increasing the "plus one" factor in the transient enhanced diffusion model from 0.01 to 1.5. Arsenic diffusion in a silicon sample implanted with 2×10^{15} cm^{-2} Si^+ can be modeled using the same plus one factor of 1.5, thereby demonstrating the consistency of the modeling. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1561996]

I. INTRODUCTION

The characterization of dopant diffusion in $Si_{1-x}Ge_x$ is important because $Si_{1-x}Ge_x$ is increasingly being used to produce devices such as heterojunction bipolar transistors and heterojunction metal–oxide–semiconductor transistors. While boron diffusion in $Si_{1-x}Ge_x$ has been reasonably well characterized,[1–3] much less research has been published on arsenic diffusion in $Si_{1-x}Ge_x$. Hu *et al.*[4] have studied segregation of arsenic in $Si_{1-x}Ge_x$, and Zou *et al.*[5] have studied the rapid thermal annealing of arsenic implanted $Si_{1-x}Ge_x$ epilayers and shown that arsenic diffusion in $Si_{1-x}Ge_x$ is enhanced compared with that in silicon.

Ion beam synthesis can be used to form $Si_{1-x}Ge_x$ heterostructures, and offers a simple way of improving device performance.[6] Lombardo *et al.*[6] have studied *npn* transistors fabricated by ion beam synthesis and found that the boron diffusion was slower than in silicon, in agreement with work on $Si_{1-x}Ge_x$ epitaxial layers.[1-3] *Pnp* transistors are also of interest for complementary bipolar circuits, and ion beam synthesis of $Si_{1-x}Ge_x$ would offer the prospect of improving the performance of the *pnp* transistor, which is inferior to that of the *npn* transistor.

In this article, we report a quantitative comparison of arsenic diffusion in $Si_{1-x}Ge_x$ layers produced using ion beam synthesis and epitaxy. It is shown that arsenic diffusion in epitaxial $Si_{1-x}Ge_x$ is increased compared with that in Si and further increased in ion beam synthesized layers.

II. EXPERIMENTAL PROCEDURE

Four (100) 0.5–1 Ω cm silicon wafers were used to investigate arsenic diffusion in $Si_{1-x}Ge_x$ produced using ion beam synthesis and epitaxy. An ion beam synthesized layer was produced in one wafer using a 2×10^{16} cm^{-2}, 100 keV $^{72}Ge^+$ implant into silicon at liquid-nitrogen temperature to give an average germanium content of 5% and an epitaxial $Si_{1-x}Ge_x$ layer was grown on a second wafer using low pressure chemical vapor deposition. The third silicon wafer was given a 60 keV, 2×10^{15} cm^{-2} Si^+ implant; the energy and dose of the Si^+ implant were chosen to give the same amorphization depth as in the Ge^+ implant. The fourth wafer was a silicon control, which was given no Ge^+ or Si^+ implants. No regrowth anneals were performed after the Ge^+ and Si^+ implants. Each wafer was then implanted with 40 keV As^+ with a dose of 1×10^{16} cm^{-2}, before oxide deposition and sawing into 15 mm^2 samples. Pieces from each wafer were then given a rapid thermal anneal of 30 s at 1025 °C in dry nitrogen.

The As and Ge profiles were determined using secondary ion mass Spectroscopy (SIMS) with an O_2^+ beam, and the experimental arsenic profiles were compared with simulated profiles obtained using TSUPREM4. The arsenic as-implanted profile was modeled using a dual Pearson distribution, with the moments chosen to give good agreement with the measured profile. Arsenic diffusion was modeled using the PD.FULL model, which includes mechanisms such as arsenic clustering, concentration dependent diffusion,[7] and transient enhanced diffusion (TED). The arsenic diffusion mechanism was assumed to be diffusion by singly negative vacancies, with an activation energy, E_a, of 4.15 eV and a pre-exponential factor, D_0, of 1.49×10^{11} μm^2/min and dif-

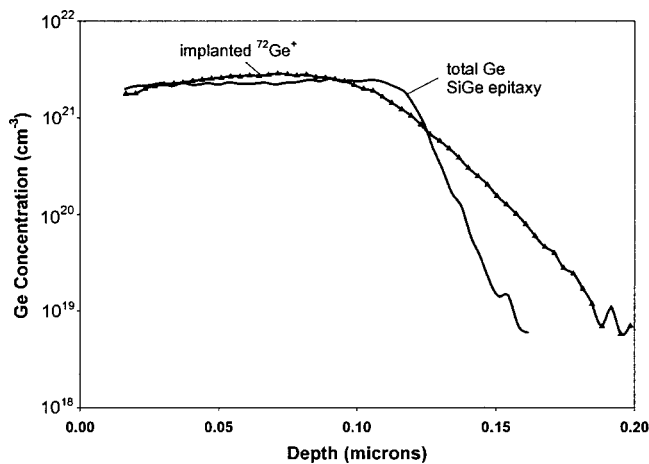[a]Author to whom correspondence should be addressed; electronic mail pa@ecs.soton.ac.uk

FIG. 1. Germanium SIMS profiles for wafers created using epitaxy and ion beam synthesis using a 100 keV 2×10^{16} cm^{-2}, 100 keV ^{72}Ge$^+$ implant.

fusion by singly negative interstitials with an activation energy of 4.15 eV and a pre-exponential factor of 3.72×10^{10} μm^2/min. For the Si control and epitaxial Si$_{1-x}$Ge$_x$ samples, singly negative interstitials were found to have little effect on the simulated profiles, whereas for the Si$^+$ and Ge$^+$ implanted samples, both singly negative vacancies and singly negative interstitials were found to influence the profiles. TED was modeled using a "plus one" model, which assumed 0.01 excess interstitials per implanted arsenic atom.[8]

III. RESULTS

Figure 1 shows the germanium SIMS profiles for the Si$_{1-x}$Ge$_x$ on Si layers produced using epitaxy and ion beam synthesis. For the Si$_{1-x}$Ge$_x$ epitaxy sample, the germanium concentration remains approximately constant down to a depth of 0.12 μm, with an average concentration of 5 at. %. For the ion beam synthesized sample, the germanium concentration peaks at a depth of 0.071 μm and has an average concentration of 5 at. % in the top 0.12 μm of the profile.
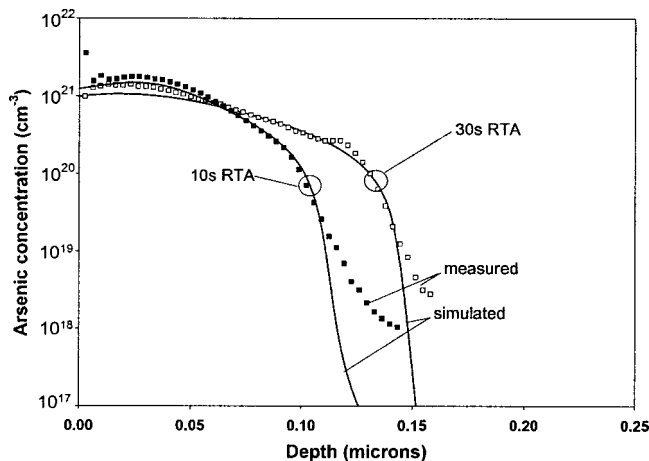

FIG. 2. Measured (SIMS) and simulated arsenic profiles for Si$_{0.95}$Ge$_{0.05}$ epitaxial layers implanted with 1×10^{16} cm^{-2} As$^+$ at 40 keV and annealed in nitrogen for 10 s or 30 s at 1025 °C. The simulated profiles were obtained using an activation energy of 4.15 eV, a pre-exponential factor of 4×10^{11} μm^2/min and a plus one model factor of 0.01.
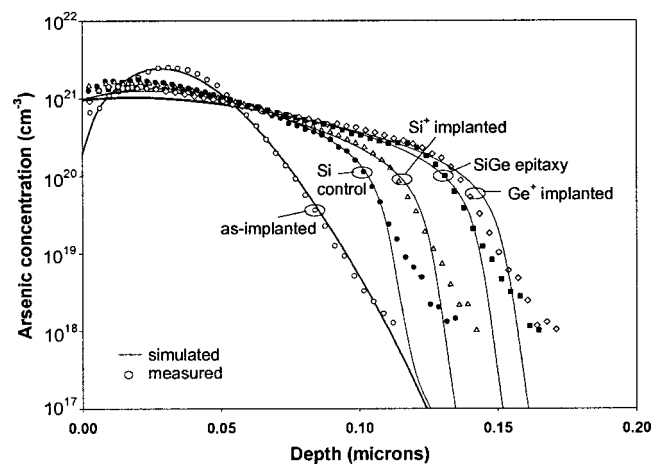

FIG. 3. Comparison of measured (SIMS) and simulated arsenic profiles in wafers implanted with 1×10^{16} cm^{-2} As$^+$ at 40 keV and annealed in nitrogen for 30 s at 1025 °C. Profiles are shown for five cases: As-implanted, Si control, Si$_{0.95}$Ge$_{0.05}$ epitaxy layer, ion beam synthesized Si$_{0.95}$Ge$_{0.05}$ layer created using a 100 keV 2×10^{16} cm^{-2} ^{72}Ge$^+$ implant, and a Si control implanted with 60 keV 2×10^{15} cm^{-2} Si$^+$. The Si control is modeled using a pre-exponential factor of 1.49×10^{11} μm^2/min and a plus one model factor of 0.01, the Si$_{0.95}$Ge$_{0.05}$ epitaxy layer using a pre-exponential factor of 4×10^{11} μm^2/min and a plus one model factor of 0.01, the Ge$^+$ implanted using a pre-exponential factor of 4×10^{11} μm^2/min and a plus one model factor of 1.5 and the Si$^+$ implanted using a pre-exponential factor of 1.49×10^{11} μm^2/min and a plus one model factor of 1.5. In all cases, an activation energy of 4.15 eV was used.

Figure 2 shows measured arsenic profiles in the epitaxial Si$_{1-x}$Ge$_x$ layer on silicon after anneals of 10 s and 30 s at 1025 °C. Also shown in Fig. 2 are modeled profiles, which were obtained using an arsenic diffusion coefficient of 5.16×10^{-15} cm^2 s^{-1}. It can be seen that both of the profiles can be reasonably well modeled using this value of diffusion coefficient.

Figure 3 compares arsenic diffusion profiles in epitaxial and ion beam synthesized Si$_{1-x}$Ge$_x$, and in Si$^+$ implanted and Si control samples after a rapid thermal anneal for 30 s at 1025 °C. Also shown in Fig. 3 is an as-implanted arsenic profile for comparison. A number of trends can be identified in these profiles. First, the arsenic diffusion in the Si$_{1-x}$Ge$_x$ epitaxy sample is significantly increased compared with that in the Si control sample. Second, the arsenic diffusion in the ion beam synthesized Si$_{1-x}$Ge$_x$ sample is increased compared with that in the Si$_{1-x}$Ge$_x$ epitaxy sample and, finally, the arsenic diffusion in the Si$^+$ implanted sample is increased compared with that in the Si control sample. Taking an arsenic concentration of 1×10^{19} cm^{-3} as a reference, the arsenic penetration depths are 0.094 μm, 0.116 μm, 0.128 μm, 0.146 μm, and 0.151 μm for the as-implanted, Si control, Si$^+$ implanted, Si$_{1-x}$Ge$_x$ epitaxy, and Si$_{1-x}$Ge$_x$ ion beam synthesized samples, respectively. The arsenic diffusion depth in the Si$_{1-x}$Ge$_x$ epitaxy sample is therefore enhanced by a factor of 1.26 compared with the Si control sample and by a factor of 1.30 in the ion beam synthesized sample.

IV. DISCUSSION

In this section, we attempt to interpret the arsenic diffusion by comparing measured and simulated arsenic profiles,

as illustrated in Fig. 3. For the Si control sample, excellent agreement is obtained between the measured and simulated arsenic profiles using a diffusion coefficient of 1.92×10^{-15} cm^2/s. This is close to the value of 3×10^{-15} cm^2/s predicted by Fair.[9]

For the Si$_{1-x}$Ge$_x$ epitaxy sample, Fig. 3 shows increased arsenic diffusion in Si$_{1-x}$Ge$_x$ compared with that in silicon. This behavior can be modeled by increasing the diffusion coefficient by a factor of 2.8, as illustrated in the simulated profile in Fig. 3. This gives a diffusion coefficient of 5.16×10^{-15} cm^2/s at a temperature of 1025 °C for arsenic in epitaxial Si$_{0.95}$Ge$_{0.05}$. Figure 3 probably represents a slight underestimate, since the arsenic penetrates beyond the flat portion of the Ge profile into the tail region.

The arsenic profiles in Fig. 3 showed that the Si$^+$ implant increased the arsenic diffusion. Since the Si$^+$ implant was performed to mimic the damage created in the substrate by a Ge$^+$ implant, it would seem logical to simulate the effect of the Si$^+$ implant by increasing the amount of damage in the simulation. This was done by increasing the plus one factor from 0.01 to 1.5. Figure 3 shows that a plus one factor of 1.5 for the Si$^+$ implanted sample gives good agreement with the measured arsenic profile.

These results indicate that the increase in arsenic diffusion in the Si$^+$ implanted Si control sample can be explained by an increase in the number of point defects. In which case, it would be expected that the Ge$^+$ implant would give rise to a similar increase in arsenic diffusion in the Si$_{1-x}$Ge$_x$. To test this hypothesis, arsenic diffusion in the Ge$^+$ implanted sample was modeled using the same plus one factor of 1.5 and by introducing diffusion by singly negative interstitials as well as diffusion by singly negative vacancies. Figure 3 shows that the simulated arsenic profile for the Ge$^+$ implanted sample is in good agreement with the measured profile, thereby demonstrating the consistency of the modeling.

Krishnamoorthy *et al.*[10] have reported increased arsenic diffusion in silicon due to damage beyond the end of range defects created by an arsenic implant, which might explain the increased arsenic diffusion seen in our ion beam synthesized Si$_{1-x}$Ge$_x$ layers. Furthermore, Jones *et al.*[11] reported that low-temperature amorphizing implants led to dislocation loops which did not hamper the flow of interstitials across the amorphous/crystalline interface. As the Si$^+$ implant in our work was performed using liquid-nitrogen cooling, this mechanism could also contribute to increased arsenic diffusion in the Si$^+$ implanted layers.

ACKNOWLEDGMENT

[1] G. H. Loechelt, G. Tam, J. W. Steele, L. K. Knoch, K. M. Klein, J. K. Watanabe, and J. W. Christiansen, J. Appl. Phys. **74**, 5520 (1993).

[2] N. Moriya, L. C. Feldman, J. S. Luftman, C. A. King, J. Bevk, and B. Feer, Phys. Rev. Lett. **71**, 883 (1993).

[3] P. Kuo, J. L. Hoyt, J. F. Gibbons, J. E. Turner, and D. Lefforge, Appl. Phys. Lett. **66**, 580 (1995).

[4] S. M. Hu, D. C. Ahlgren, P. A. Ronsheim, and J. O. Chu, Phys. Rev. Lett. **67**, 1450 (1991).

[5] L.-F. Zou, Z. G. Wang, D. Z. Sun, T. W. Fan, X. F. Liu, and J. W. Zhang, Nucl. Instrum. Methods Phys. Res. B **122**, 639 (1997).

[6] S. A. Lombardo, V. Privtera, A. Pinto, G. La Rosa, and S. U. Campisano, IEEE Trans. Electron Devices **45**, 1531 (1998).

[7] A. F. W. Willoughby, Rep. Prog. Phys. **41**, 1665 (1978).

[8] R. F. Lever, J. M. Bonar and A. F. W. Willoughby, J. Appl. Phys. **83**, 1988 (1998).

[9] R. B. Fair, in *Impurity Doping Processes in Silicon,* edited by F. F. Y. Wang (North–Holland, New York, 1981), Chap. 7.

[10] V. Krishnamoorthy, K. Moller, K. S. Jones, D. Venables, J. Jackson, and L. Rubin, J. Appl. Phys. **84**, 5997 (1998).

[11] K. S. Jones, K. Moller, J. Chen, M. Puga-Lambers, B. Freer, J. Berstein, and L. Rubin, J. Appl. Phys. **81**, 6051 (1997).