

Dislocation loops in silicon-germanium alloys: The source of interstitials

R. T. Crosby,^{a)} K. S. Jones, M. E. Law, and L. Radic
 SWAMP Center, University of Florida, Gainesville, Florida 32611

P. E. Thompson
 Code 6812, Naval Research Laboratory, Washington, DC 20375

J. Liu
 Varian Semiconductor Equipment Associates, Gloucester, Massachusetts 01930

(Received 27 May 2005; accepted 8 September 2005; published online 3 November 2005)

The relationships between extended defect evolution and boron diffusion in $\text{Si}_{0.77}\text{Ge}_{0.23}$ have been investigated. A SiGe structure was grown by molecular beam epitaxy with a 3×10^{18} atoms/cm³ boron marker layer positioned 0.50 μm below the surface. Samples were ion implanted with 60 keV Si^+ at a dose of 1×10^{14} atoms/cm² and subsequently annealed at 750 °C for various times. The evolution of extended defects in the near surface region was monitored with plan-view transmission electron microscopy. Secondary ion mass spectroscopy concentration profiles facilitated the characterization of boron diffusion. Boron experiences transient enhanced diffusion regulated by the dissolution of dislocation loops. The maximum diffusion enhancement in $\text{Si}_{0.77}\text{Ge}_{0.23}$ is less than that observed in pure Si. © 2005 American Institute of Physics. [DOI: 10.1063/1.2123389]

With SiGe growing as a mainstream component of today's complementary metal-oxide-semiconductor design, dopant diffusion and defect studies of relaxed $\text{Si}_{1-x}\text{Ge}_x$ alloys are crucial to the performance optimization SiGe-based devices. It is well known that upon annealing implant damage in Si, the injected interstitials drive transient enhanced diffusion (TED).¹⁻³ To rule out the effects of doping and variations in damage, Si implantation into buried B marker layers was used to study TED.⁴ Later, researchers would correlate the observed TED of B to defect evolution using plan-view transmission electron microscopy (PTM).² Under conventional annealing and nonamorphizing implantation conditions, these excess interstitials will form subthreshold defects (i.e., {311} defects, and dislocations loops) around the projected range of the implant where the interstitial supersaturation is the highest.⁵⁻⁷ TED in Si under the amorphization threshold is known to be governed by the evolution of {311} defects.^{2,3,7}

Recently, it has been shown that under these conventional practices, {311} defects were observed in SiGe with Ge compositions less than or equal to 5%. At Ge compositions greater than or equal to 25%, interstitials agglomerated into dislocation loops. These dislocation loops exemplify stability at Ge fractions of 25% and 35%,⁸ where Si is proposed to switch diffusion paths.⁹ The collapse of the {311} defect configuration between 5% and 25% is primarily due to the reduced binding energy of the alloy.⁸

Early experiments have confirmed that B diffuses less in SiGe (Refs. 10 and 11) than in pure Si due to preferential Ge-B bonding^{12,13} and strain compensation.¹¹ Under interstitial injection from annealing in a dry O₂ ambient, it has been determined that B diffusion is interstitially mediated in Si-rich alloys.¹⁴⁻¹⁶ For full integration of SiGe heterostructures, it will be technologically important to address the diffusion behavior under interstitial supersaturation induced by ion-implantation. As, P, (Refs. 17 and 18) and B (Ref. 19) experience enhanced diffusion in SiGe, but these experiments

lack the correlation between TED and extended defect formation necessary for a complete understanding of interstitial supersaturation and dopant diffusion. The nature of point defect evolution and the related B diffusion in SiGe will be examined using similar tactics used to characterize these interactions in pure Si.

$\text{Si}_{0.77}\text{Ge}_{0.23}$ of constant composition was grown to a thickness $\sim 1 \mu\text{m}$ on top of relaxed $\text{Si}_{0.80}\text{Ge}_{0.20}$ virtual substrates via molecular beam epitaxy methodology. At 0.50 μm below the surface, a 10 nm (full width at half maximum) boron marker layer was grown with a peak concentration of $3.0 \times 10^{18} \text{ cm}^{-3}$. This layer will be used to monitor disturbances in the point defect equilibrium induced by a surface implant and annealing. A subsequent 0.50 μm undoped layer of $\text{Si}_{0.77}\text{Ge}_{0.23}$ was grown on top of the boron marker layer. Confining the study to subthreshold defect evolution, the structure was implanted with a nonamorphizing (as verified by cross-sectional TEM) 60 keV, $1 \times 10^{14} \text{ cm}^{-2}$ Si^+ implant with a projected range of 65 nm. The samples were subsequently furnace annealed in a N₂ ambient at 750 °C. PTM was used to quantify defect evolution, and secondary ion mass spectroscopy (SIMS) was used to measure the diffusion of B in the marker layer with and without Si^+ implant.

It should be noted that the $\text{Si}_{0.77}\text{Ge}_{0.23}$ containing the B marker has a Ge composition slightly higher than the underlying virtual $\text{Si}_{0.80}\text{Ge}_{0.20}$ as verified by high resolution x-ray diffraction. Auger electron spectroscopy confirmed that the Ge atomic percent in the B-doped overlayer is $23\% \pm 1\%$. At most, this amounts to a compressive film strain of 0.10%. These strain levels have been shown to be too insignificant to alter the diffusion of B in SiGe.¹²

The B diffusion profiles of the Si^+ -implanted $\text{Si}_{0.77}\text{Ge}_{0.23}$ structures are shown in Fig. 1. Without Si^+ implantation, B exhibits intrinsic behavior diffusing relatively small distances after thermal cycles of 750 °C for 30 min and 2 h. The diffusivity of B in $\text{Si}_{0.77}\text{Ge}_{0.23}$ at 750 °C are comparable to values extrapolated from the findings of Zangenberg *et al.* suggesting that B would diffuse 2.5 nm after 30 min of annealing and 6 nm after 2 h of annealing.²⁰ From the profile of

^{a)}Electronic mail: tecz@ufl.edu

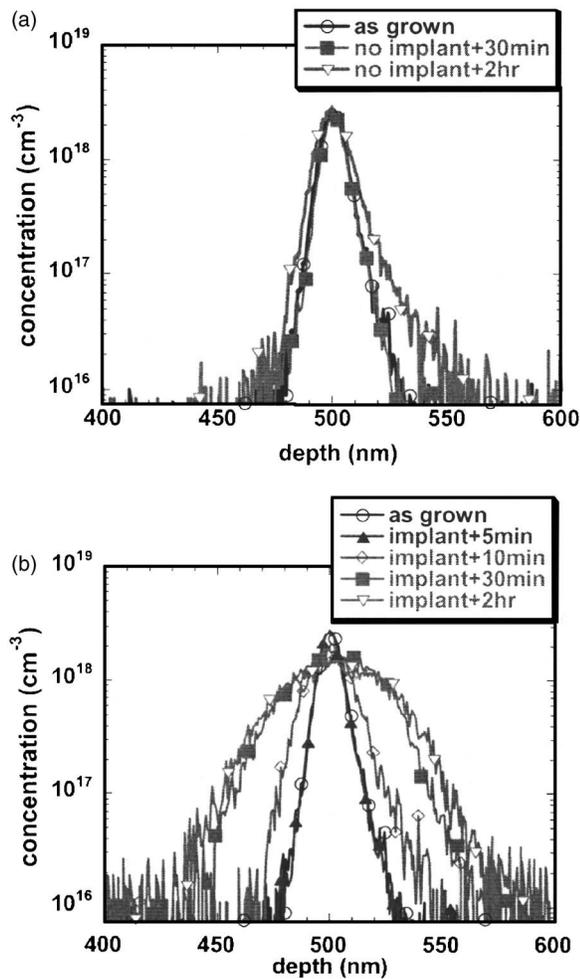


FIG. 1. SIMS profiles of B marker in SiGe annealed at 750 °C (a) without and (b) with a 60 keV, $1 \times 10^{14} \text{ cm}^{-2} \text{ Si}^+$.

the sample annealed at 750 °C for 2 h, an equilibrium diffusivity of $7.8 \times 10^{-18} \text{ cm}^2/\text{s}$ for B in $\text{Si}_{0.77}\text{Ge}_{0.23}$ was extracted. After ion implantation, the nature of B diffusion is significantly altered. After 5 min, there exist no measurable diffusion, but by 10 min, the profiles have broadened significantly. The profile broadening of the samples annealed for 10 and 30 min reveal increases in diffusivity by factors of 130 and 118, respectively, by virtue of the $x=2\sqrt{Dt}$ relation. The diffusion of B is enhanced by the presence of excess interstitials after the repair of implant damage. The enhancement drops off significantly to a value of 42 after 2 h of annealing suggestive of a similar transient behavior observed with enhanced B diffusion in Si after implantation.^{21,22} The initial burst of B-TED resulting from the same implant in Si is apparent after a 740 °C rapid thermal annealing with a dwell time of 2 s and is three orders of magnitude higher than the effective enhanced diffusivity measured after a 750 °C anneal for 10 min in $\text{Si}_{0.77}\text{Ge}_{0.23}$. Despite the lower melting temperature and the two orders of magnitude difference in thermal budget, B exhibits a lower diffusivity after implantation in $\text{Si}_{0.77}\text{Ge}_{0.23}$ than in pure Si.

Weak beam dark-field g_{220} PTEM was used to monitor the evolution of extended defects in $\text{Si}_{0.77}\text{Ge}_{0.23}$ shown in Fig. 2. These processing conditions are known to produce $\{311\}$ defects in Si that dissolve trapped interstitials and drive TED. Consistent with previous observations,⁸ stable dislocation loops are the only observable subthreshold defect. Due to the lower binding energy and lattice distortion when incorporating Ge atoms, the rigid confinements of the $\{311\}$ defect configuration²³ become increasingly more unstable. Interesting to note, the defect density appears to be significantly higher during the earlier phases of annealing.

To correlate the observed B diffusion with defect dissolution, time-averaged diffusivity enhancement at discrete in-

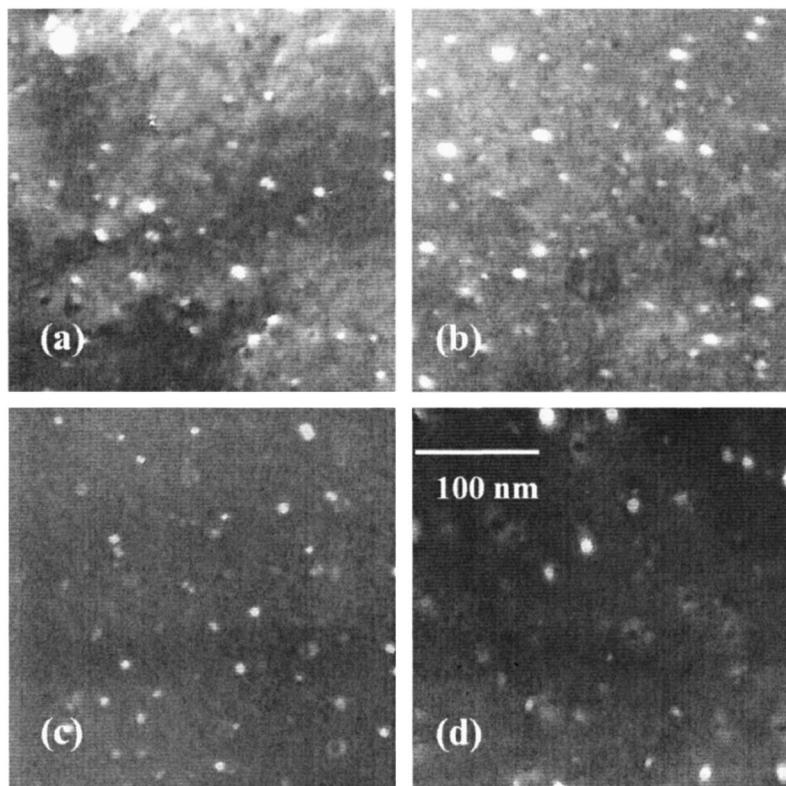


FIG. 2. PTEM images of SiGe implanted with 60 keV, $1 \times 10^{14} \text{ cm}^{-2} \text{ Si}$ and annealed at 750 °C for (a) 5, (b) 10, (c) 30, and (d) 120 min.

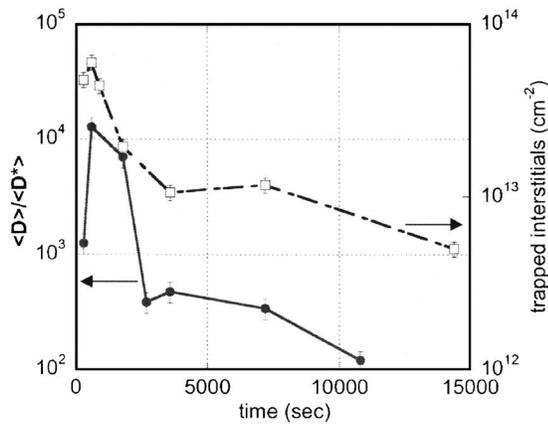


FIG. 3. Trapped interstitial and time-averaged diffusivity enhancement as a function of anneal time for SiGe implanted with 60 keV, 1×10^{14} cm $^{-2}$ Si and annealed at 750 °C.

tervals are plotted with trapped interstitial density in Fig. 3. The trapped interstitials reveal two regimes of defect dissolution corresponding well with observed TED. By exponentially fitting (i.e., $C = C_0 \exp[-kt]^2$) the data from 5 to 30 min and then 30 min to 4 h, decay times of the two separate regimes were calculated. The decay time of trapped interstitials during fast dissolution in the earlier parts of the anneal is 30.4 min; while the decay time for slow dissolution after 30 min of annealing is 183 min. Dislocation loops nucleate within 5 min, and nearly all excess interstitials are clustered; hence, there exist no discernible TED. By 10 min, dislocation loops coarsen, and the initial phases of dissolution are marked by the strong TED of B. By 30 min, trapped interstitials have dissolved significantly, and enhancement is still high. After 30 min, the enhancement drops off two orders of magnitude. This behavior relates directly back to the trapped interstitials driving diffusion. Annealing more than 30 min reveals the slow dissolution of trapped interstitials from dislocation loops.

Dislocation loops in Si $_{0.77}$ Ge $_{0.23}$ trap interstitials that drive B-TED much like {311} defects in Si. Consequently, as long as dislocation loops are present in Si $_{0.77}$ Ge $_{0.23}$, the enhancement of B diffusion will persist. Also TED is maximized near the beginning of the anneal, correlating with interstitial supersaturation. As the interstitial supersaturation decreases with annealing, so does TED.

B diffusion in Si $_{0.8}$ Ge $_{0.2}$ is mediated by interstitials¹⁴ and possibly by a similar kick-out mechanism proposed for B diffusion in Si which may become gradually more unfavorable in the presence of longer, more floppy Ge bonds.²⁴ To specify the kick-out of B into an interstitial position by the presence of Ge is plausible; however, this complex is immobile, and the kick-in of B back into a substitutional position is unfavorable. The interstitials available for the formation of mobile B–I pairs are mostly Si-type because Ge interstitial formation is more unfavorable than Si interstitial formation.

With alloying, there are less Si interstitials to drive B diffusion, and the presence of Ge serves as an additional trap for B (Refs. 12 and 13) and reduces the migration of interstitials.^{9,24} Implanting excess interstitials generates Si interstitials sufficient for B binding, kick-out, and accelerated pair travel. These implanted interstitials agglomerate into dislocation loops, and upon dissolution, form the B–I complexes necessary for B diffusion. The reduced interstitial migration in the presence of Ge is made apparent by the delayed onset of TED in Si $_{0.77}$ Ge $_{0.23}$.

In summary, dislocation loops are the only observed sub-threshold defect in Si $_{0.77}$ Ge $_{0.23}$ upon annealing. In the initial stages of annealing, these defects dissolve more quickly. A slower dissolution of trapped interstitials is observed when annealing more than 30 min at 750 °C. The trapped interstitials that drive B-TED are maximum after 10 min of annealing and drops off steadily after 30 min.

- ¹N. E. B. Cowern, K. T. F. Janssen, and H. F. F. Jos, *J. Appl. Phys.* **68**, 6191 (1990).
- ²D. J. Eaglesham, P. A. Stolk, H.-J. Gossmann, and J. M. Poate, *Appl. Phys. Lett.* **65**, 2305 (1994).
- ³P. A. Stolk, H.-J. Gossmann, D. J. Eaglesham, and J. M. Poate, *Nucl. Instrum. Methods Phys. Res. B* **96**, 187 (1995).
- ⁴P. Packan, Ph. D. thesis, Stanford University, Palo Alto, CA, 1991.
- ⁵W. Vandervorst, D. C. Houghton, F. R. Shepherd, M. L. Swanson, H. H. Plattner, and G. J. C. Carpenter, *Can. J. Phys.* **63**, 863 (1985).
- ⁶K. S. Jones, S. Prussin, and E. R. Weber, *Appl. Phys. A* **45**, 1 (1988).
- ⁷C. S. Rafferty, G. H. Gilmer, M. Jaraiz, D. Eaglesham, and H.-J. Gossmann, *Appl. Phys. Lett.* **68**, 2395 (1996).
- ⁸R. T. Crosby, K. S. Jones, M. E. Law, A. Nylandsted Larsen, and J. Lundgaard Hansen, *Mater. Sci. Semicond. Process.* **6**, 205 (2003).
- ⁹A. Strohm, T. Voss, W. Frank, P. Laitinen, and J. Raisanen, *Z. Metallkd.* **93**, 737 (2002).
- ¹⁰P. Kuo, J. L. Hoyt, J. F. Gibbons, J. E. Turner, R. D. Jacowitz, and T. I. Kamins, *Appl. Phys. Lett.* **62**, 612 (1992).
- ¹¹N. Moriya, L. C. Feldman, H. S. Luftman, C. A. King, J. Bevk, and B. Freer, *Phys. Rev. Lett.* **71**, 883 (1993).
- ¹²P. Kuo, J. L. Hoyt, and J. F. Gibbons, *Appl. Phys. Lett.* **66**, 580 (1995).
- ¹³R. F. Lever, J. M. Bonar, and A. F. W. Willoughby, *J. Appl. Phys.* **83**, 1988 (1998).
- ¹⁴T. C. W. Fang, T. T. Fang, P. B. Griffin, and J. D. Plummer, *Appl. Phys. Lett.* **68**, 2085 (1996).
- ¹⁵J. M. Bonar, A. F. W. Willoughby, A. H. Dan, B. M. McGregor, W. Lerch, D. Loeffelmacher, G. A. Cooke, and M. G. Dowsett, *J. Mater. Sci.: Mater. Electron.* **12**, 219 (2001).
- ¹⁶P. M. Fahey, P. B. Griffin, and J. D. Plummer, *Rev. Mod. Phys.* **61**, 289 (1989).
- ¹⁷S. Eguchi, J. J. Lee, S. J. Rhee, D. L. Kwong, M. L. Lee, E. A. Fitzgerald, I. Aberg, and J. L. Hoyt, *Appl. Surf. Sci.* **224**, 59 (2004).
- ¹⁸S. Eguchi, J. L. Hoyt, C. W. Lietz, and E. A. Fitzgerald, *Appl. Phys. Lett.* **80**, 1743 (2002).
- ¹⁹C. C. Wang, T. Y. Huang, Y. M. Sheu, R. Duffy, A. Heringa, N. E. B. Cowern, P. B. Griffin, and C. H. Diaz, *Proc. Inter. Conf. Simul. Semic. Proc. Dev.*, 2004.
- ²⁰N. Zangenber, J. Fage-Pedersen, J. Lundgaard Hansen, and A. Nylandsted Larsen, *J. Appl. Phys.* **94**, 25901 (2000).
- ²¹S. Solmi, F. Baruffaldi, and R. Canteri, *J. Appl. Phys.* **69**, 2135 (1991).
- ²²A. E. Michel, W. Rausch, P. A. Ronsheim, and R. H. Kastl, *Appl. Phys. Lett.* **51**, 487 (1987).
- ²³T. Y. Tan, *Philos. Mag. A* **44**, 101 (1981).
- ²⁴L. Wang, P. Clancy, and C. S. Murthy, *Phys. Rev. B* **70**, 165206 (2004).