Boron diffusion in amorphous silicon-germanium alloys

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The effect of Ge alloying on B diffusion in amorphous $Si_{1-x}Ge_x$ alloys is reported for $x=0-0.24$. The diffusivity was not observed to exhibit any transient decay. The diffusivity decreases with increasing Ge concentration. The activation energy for B diffusion appears to increase from 2.8 eV for amorphous Si to 3.6 eV for amorphous $Si_{0.76}Ge_{0.24}$. It is suggested that, in these alloys, Ge distorts the amorphous Si network thereby increasing B trapping by Si. © *2008 American Institute of Physics*. [DOI: 10.1063/1.2919085]

B is the most common ion implanted dopant used for the formation of *p*-type regions in Si because of its high solubility and low ionization energy. Preamorphization of Si prior to B implantation has several advantages for the fabrication of ultrashallow junctions including suppression of ion channeling and increased activation of B due to dopant incorporation during low-temperature solid phase epitaxial regrowth (SPER) of the amorphous layer.[1] However, prior to the completion of SPER, B can diffuse in the amorphous phase. With the increased use of millisecond annealing, this diffusion can become a significant fraction of the total diffusion observed. Previous studies have shown that B diffusion in the amorphous phase is approximately four orders of magnitude faster than that observed in crystalline Si at the same temperature.[2,3]

Strained SiGe is currently being used to enhance hole mobility in *p*-channel metal-oxide-semiconductor devices.[4] It is therefore important to understand how B diffusion is affected by alloy composition. In strain-relaxed crystalline SiGe alloys, the effect of Ge on B diffusion is inconclusive.[5,6] While it appears that Ge incorporation decreases B diffusivity, the relative extent and cause of this effect is uncertain. Kuo *et al.* proposed that B diffusivity in strain-relaxed SiGe alloys is a function of Ge content.[5] Zangenberg *et al.* suggested the formation of an immobile Ge–B complex that dominates over the diffusion coefficient, in effect rendering the B diffusion independent of Ge content.[6] However, recent calculations report a binding energy between Ge and B in the crystalline phase prohibitively small to account for the decrease in B diffusion and instead attributes the retardation of B to an increase in migration energy upon Ge incorporation.[7] Previous work has shown no dependence of B diffusion on Ge concentration for amorphous SiGe alloys with compositions of Ge <12 at. %.[8] In this work, the effect of Ge concentration on the diffusion of B in the amorphous SiGe phase for Ge compositions between 12 and 24 at. % is studied over a wide temperature range in order to clearly discern the affect of alloying.

Strain-relaxed $Si_{1-x}Ge_x$ layers ($x=0.12$, 0.18, and 0.24) were grown on (001) Si substrates using reduced pressure chemical vapor deposition. The Si control used was (001)

oriented bulk wafers. Samples were preamorphized from the surface to a depth of approximately 850 nm, by cooling them to approximately 77 K and implanting with Si^+ ions (5×10^{10} ions/cm^2 at 500 keV, plus 1×10^{15} ions/cm^2 at 95 keV). The samples then received a B^+ implant of 1×10^{15} ions/cm^2 at 500 eV. Postimplant annealings were conducted in a quartz tube furnace under N_2 ambient. The annealing times and temperatures were chosen so as to limit the diffusion measurements to only the amorphous phase (i.e., prior to interaction with the advancing amorphous/crystalline interface).[9] Cross-sectional transmission electron microscopy was used to measure amorphous layer depths before and after annealing to confirm that the advancing amorphous/crystalline interface had not reached the B profile. Secondary ion mass spectroscopy (SIMS) profiles were collected using an O_2^+ beam with net impact energy of 600 eV and a beam current of 180 nA. In order to estimate B diffusivity, the diffusion length was measured at a B concentration of 3×10^{19} and 3×10^{18} cm^{-3} and equated to $2\sqrt{(D_B t)}$. The activation energy and preexponential factor were derived from an Arrhenius expression of the diffusivity as a function of temperature.

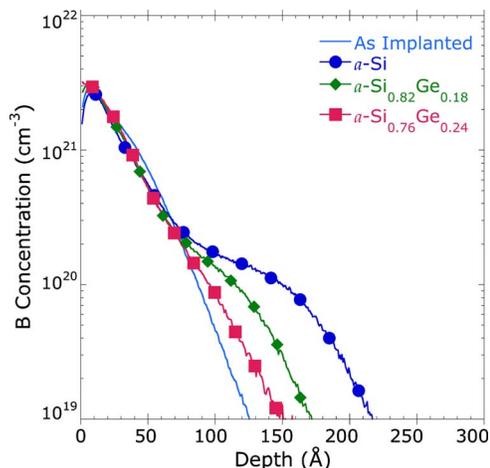Figure 1 shows the B dopant profiles for amorphous

FIG. 1. (Color online) SIMS profiles of B motion in the as-implanted sample and after annealing at 500 °C for 25 h in *a*-Si, *a*-$Si_{0.82}Ge_{0.18}$, and *a*-$Si_{076}Ge_{0.24}$. SIMS profile for B in *a*-$Si_{0.88}Ge_{0.12}$ is omitted for clarity.
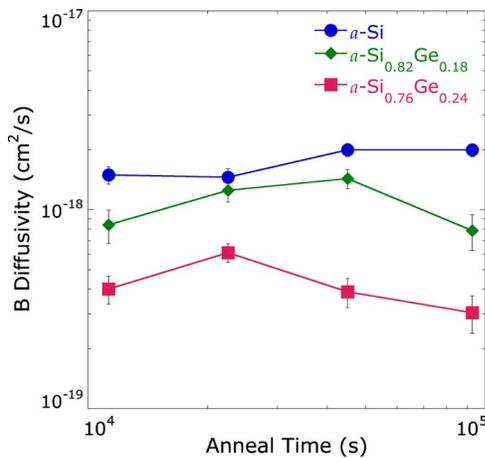
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FIG. 2. (Color online) B diffusivites for a-Si, a-Si$_{0.82}$Ge$_{0.18}$, and a-Si$_{076}$Ge$_{0.24}$ at 500 °C for a series of annealing times. B diffusivities for a-Si$_{0.88}$Ge$_{0.12}$ are omitted for clarity.

FIG. 3. (Color online) Arrhenius plot of B diffusivities for a-Si, a-Si$_{0.88}$Ge$_{0.12}$, a-Si$_{0.82}$Ge$_{0.18}$, and a-Si$_{076}$Ge$_{0.24}$. Annealing times ranged from 0.2 to 25 h.

(a-) Si, a-Si$_{0.82}$Ge$_{0.18}$, and a-Si$_{0.76}$Ge$_{0.24}$ following implantation and annealing at 500 °C for 25 h. After annealing, the B profiles show a characteristic "knee" that is consistent with the presence of an immobile fraction above concentrations of approximately 2×10^{20} cm^{-3} and a second mobile fraction below this value. This is indicative of B clustering and the B diffusion upon annealing is concentration dependent.[10] For a-Si, the B clustering process is believed to very rapidly occur at these temperatures. For the a-Si$_{1-x}$Ge$_x$ alloys, there is an obvious reduction in the diffusion length of the mobile fraction as the Ge concentration in contrast for previous results for Ge <12 at. %.[8]

Recent results report that B exhibits a transient enhancement in diffusivity in a-Si.[11,12] This transient decays approximately one order of magnitude over 0.25 h for annealing temperatures between 600 and 650 °C before stabilizing. However, at 450 and 500 °C, very little transient behavior was observed.[11] This experiment focused on annealing temperatures between 500 and 600 °C for annealing times between 0.2 and 24 h. B diffusivity was estimated for a series of anneal times at 500 °C for varying Ge content at a B concentrations of 3×10^{19} and 3×10^{18} cm^{-3}. The results plotted in Fig. 2 exhibit no transient behavior. This is consistent with previous observations for B diffusion in pure a-Si at these lower temperature time intervals.[3,8]

A least squares fit was made to the diffusivity at each temperature. Figure 3 shows an Arrhenius plot of the B diffusivity as a function of $1/T$ for varying Ge concentrations. Previous work reported B diffusivity in a-Si to be 2.6×10^{-16} cm^2/s at 600 °C and 3×10^{-17} cm^2/s at 550 °C, which compares well with this data.[13,3] It can be seen that incorporating Ge to the a-Si matrix at Ge concentrations above 12 at. % retards B diffusion.

For each a-Si$_{1-x}$Ge$_x$ alloy studied, the activation energy for B diffusion ($E_a^{\ B}$) and the diffusion coefficient (D_o) were determined by fitting the curve with a standard Arrhenius relationship, $D=D_o \exp(-\Delta E_a^{\ B}/kT)$. These results are shown in Table I. The activation energy for B diffusion shows an increase with increasing Ge content. It appears the increase in activation energy for B diffusion is primarily responsible for the decrease in B diffusion with increasing Ge content despite the increase in the diffusion coefficient as shown in Table I. Recent molecular dynamics (MD) simulations of B
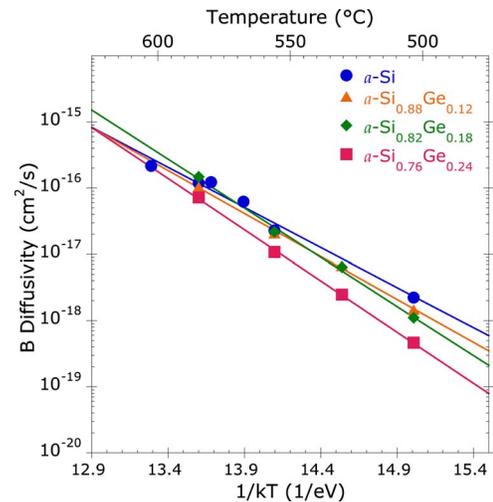
diffusion in a-Si predicts an activation energy for B diffusion of 3.0 eV, which is dependent on the capture and release of dangling bonds.[11] Other simulation results suggest an additive kinetic barrier for B diffusion composed of a formation energy for mobile B of 1.5 eV and a migration energy of 0.6 eV for B in a-Si.[14] However, there are no reported MD simulations of how Ge alloying effects the B diffusion in a-Si.

One possible reason for the decrease in B diffusivity with increasing Ge concentration is the increased trapping of B. a-SiGe is believed to be a tetrahedral network with additional three- and fivefold coordinated atoms, consistent with networks observed in pure a-Si and pure a-Ge.[15] As Ge is initially added to the a-Si matrix, its presence on one of the second or third nearest neighbor sites may cause enough distortion to make it easier to form a trap site. When the Ge concentration reaches 20%, the tetrahedral coordination of the amorphous matrix results in a first nearest neighbor impact by Ge on the network. The distortion by Ge to the random network structure could therefore increase trapping of B by Si thereby increasing the activation energy for B diffusion.

In conclusion, incorporation of Ge in a-Si at concentrations between 0 and 24 at. % has been shown to significantly decrease B diffusion in a-SiGe alloys when the Ge concentration exceeds 12 at. %. For the time intervals studied, no transient behavior was observed. The decrease in diffusivity with increasing Ge concentration arises from an increase in the activation energy. The addition of Ge may increase the kinetic barriers of the dangling bonds or increase the formation or migration energy for mobile B. Additional MD simulations may help explain the observed Ge dependence.

TABLE I. Activation energy for B diffusion and diffusion coefficient from Arrhenius fits to the B diffusivity data for a-Si$_{1-x}$Ge$_x$ alloys.

			x	
	0	0.12	0.18	0.24
$E_a^{\ B}$ (eV)	2.8 ± 0.2	2.8 ± 0.1	3.4 ± 0.1	3.6 ± 0.1
D_o (cm^2/s)	3.5	4.4	2.1×10^4	7.4×10^4

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