AIP | Applied Physics Letters

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Citation: Applied Physics Letters **105**, 042113 (2014); doi: 10.1063/1.4892079
View online: http://dx.doi.org/10.1063/1.4892079
View Table of Contents: http://scitation.aip.org/content/aip/journal/apl/105/4?ver=pdfcov
Published by the AIP Publishing

APPLIED PHYSICS LETTERS **105**, 042113 (2014)

Concentration-dependent diffusion of ion-implanted silicon in $In_{0.53}Ga_{0.47}As$

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(Received 19 May 2014; accepted 22 July 2014; published online 31 July 2014)

In contrast to prior reports, evidence of concentration-dependent diffusion is reported for Si implanted $In_{0.53}Ga_{0.47}As$. The Fickian and concentration-dependent components of diffusivities were extracted using the Florida object oriented process and device simulator. The migration energy for silicon diffusion in $In_{0.53}Ga_{0.47}As$ was calculated to be 2.4 and 1.5 eV for the Fickian and concentration dependent components of diffusion, respectively. A lack of change in diffusivities at given anneal temperatures suggest that transient-enhanced diffusion has not occurred. Due to these findings, silicon diffusion at high doping concentrations ($>1 \times 10^{20}\,cm^{-3}$) should be better characterized and understood for future complimentary metal-oxide semiconductor applications. © *2014 AIP Publishing LLC*. [http://dx.doi.org/10.1063/1.4892079]

As device scaling continues towards sub-10 nm nodes, understanding dopant diffusion and activation at this scale is of great importance, in silicon and in new material systems. III-V materials are promising candidates for future devices and features, such as fin-shaped field effect transistors (finFETs), due to their excellent electron mobilities.[1–3] In III-As related systems, silicon is considered to be an attractive n-type dopant due to its reportedly low diffusivity and good activation relative to heavier, more damaging species.[4] The goal of this study is to explore the diffusion of Si in $In_{0.53}Ga_{0.47}As$ after elevated temperature implantation.

A 10 keV, $5 \times 10^{14}\,cm^{-2}$ Si^+ dose was implanted at 80 °C and 7° tilt into a 300 nm [001] layer of $In_{0.53}Ga_{0.47}As$ grown by metal organic chemical vapor deposition (MOCVD) onto InP. Room temperature implants can amorphize $In_{0.53}Ga_{0.47}As$, resulting in poor electrical and structural properties.[5,6] It was experimentally determined that implanting at a temperature of 80 °C avoided amorphization and thus the condition was also used for this study.[7] All samples were capped with 15 nm of Al_2O_3, to prevent sample degradation and arsenic loss. The anneal conditions ranged from 550 °C to 750 °C for several durations between 5 min and 18 h in a tube furnace with Ar ambient. All of the secondary ion mass spectrometry (SIMS) profiles were obtained using a 350 eV Cs^+ primary beam for sputtering of the sample. SIMS concentrations and depths were calibrated and confirmed through dose integration and profilometry.

Several prior studies have reported negligible diffusion of silicon in $In_{0.53}Ga_{0.47}As$.[8–11] Fig. 1 shows that the 10 keV, $5 \times 10^{14}\,cm^{-2}$ Si^+ implant at 80 °C exhibits significant diffusion upon annealing at 600–750 °C. The plateau or "shoulder" of the profile is very characteristic of concentration-dependent diffusion, which becomes more pronounced with increased anneal duration. Most of the Si redistribution occurred $\sim 3–4 \times 10^{19}\,cm^{-3}$ concentration, whereas prior works studying Si diffusion in implanted $In_{0.53}Ga_{0.47}As$ had peak concentrations below that threshold, or used significantly higher implant energies.[8–10] There also appears to be a lack of temperature dependence for Si solubility, as suggested by the relatively fixed concentration of the plateaus of samples at different annealing temperatures.

In this study, experimental diffusivities were extracted using FLOOXS (Florida Object Oriented Process and Device Simulator). The main function used to fit the SIMS profiles is included in the following equation:

$$D = D_f + D_c\left(\frac{C}{10^{19}}\right)^n, \tag{1}$$

where the variables D_f, D_c, and n are the Fickian component, concentration-dependent component, and power of concentration dependence, respectively. C is the mobile concentration of silicon at a given location in the sample. A value of 10^{19} was a chosen sensitivity parameter for concentration-dependence, because it was the same order of magnitude as the profile plateau concentrations. The commonly used free carrier concentration over intrinsic carrier concentration term $\left(\frac{n}{ni}\right)$ was not implemented in the model due to the fact that the electrical solubility was calculated to be $\sim 1.7 \times 10^{19}\,cm^{-3}$ at 750 °C, using measured active sheet numbers and Si SIMS profile integration as described previously.[12] The net electrical solubility was significantly lower than the total mobile Si concentrations ($\sim 3.0 \times 10^{19}\,cm^{-3}$) during anneals. This discrepancy would suggest there is a significant mobile, yet electrically inactive, fraction of Si in this system.

Except for the 550 °C anneals (with n = 2), most of samples exhibited a strong concentration-dependence for silicon diffusion, indicated by very sharp profiles (n = 4). Examples of profile fits obtained with the aforementioned fitting parameters in FLOOXS are included in Fig. 2. The concentration dependent diffusivities were smaller than Fickian diffusivities due to the high degree of concentration dependence (n = 4, in Eq. (1)) for most samples.

Both Fickian and concentration-dependent diffusivities were plotted for their respective migration energies separately. Fig. 3 shows migration energies of the concentration dependent and Fickian components which were determined to be 2.4 and 1.5 eV, respectively.

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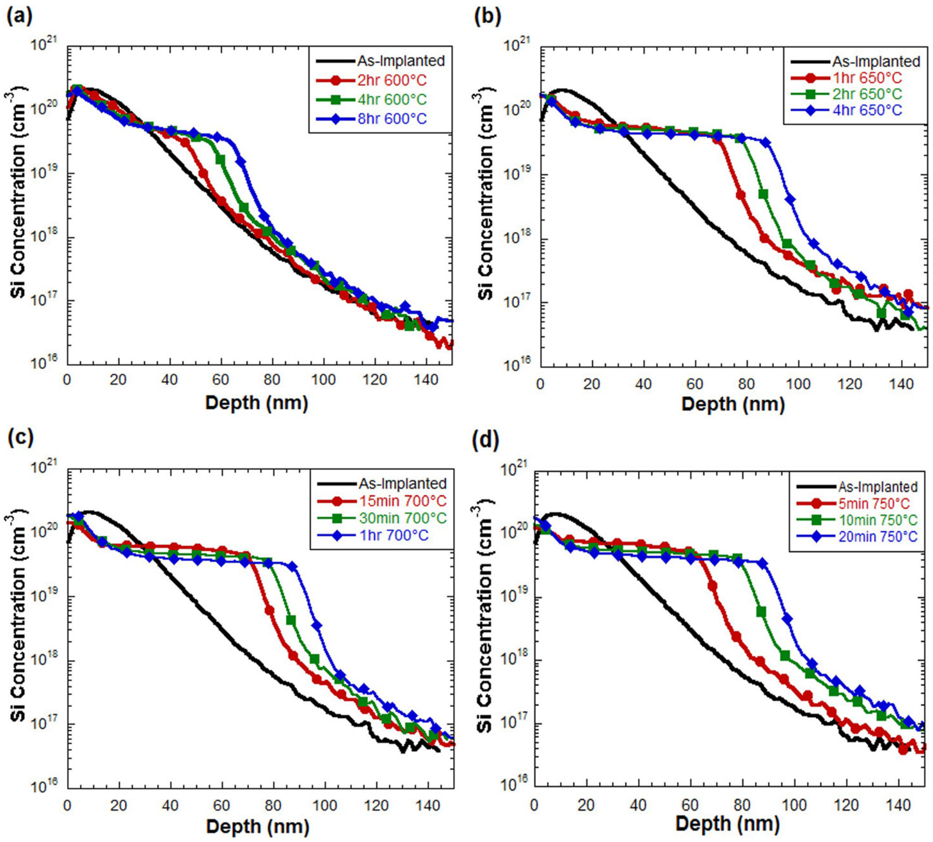

FIG. 1. SIMS profiles of as-implanted and annealed 10 keV $5 \times 10^{14}\,\mathrm{cm}^{-2}$ Si implants for (a) 600 °C, (b) 650 °C, (c) 700 °C, and (d) 750 °C furnace anneals at varying times.

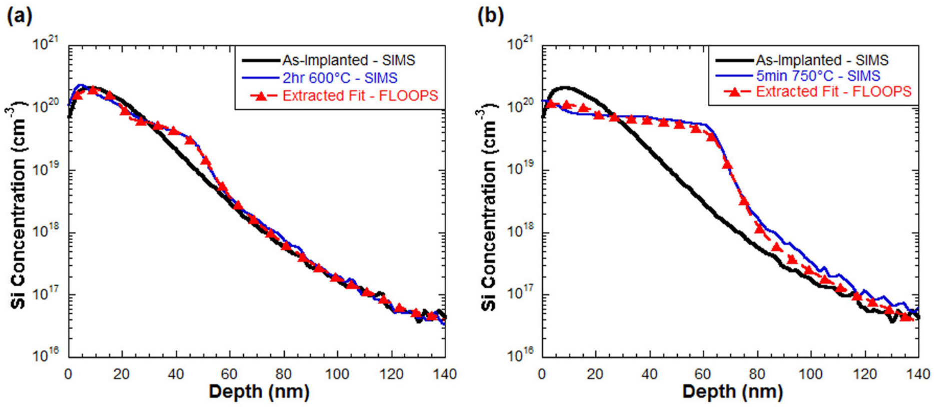

FIG. 2. Comparison of measured SIMS profile with fits generated with FLOOXS for (a) 2 h, 600 °C ($n = 2$) and (b) 5 m, 750 °C ($n = 4$) furnace anneals.

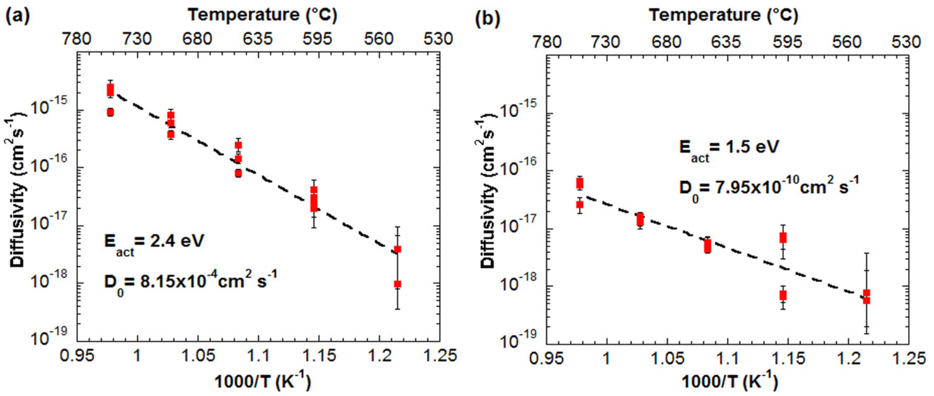

FIG. 3. Diffusivity as a function of inverse temperature for furnace anneals ranging from 550 to 750 °C, for (a) Fickian and (b) concentration-dependent diffusion components. Extracted migration energies and pre-factors are inset.

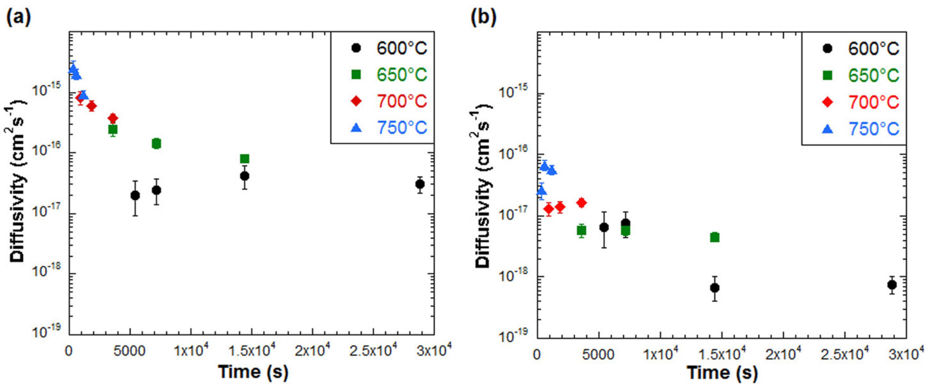

FIG. 4. Diffusivity as a function of annealing time for (a) Fickian and (b) concentration-dependent diffusion components.

Silicon is a known vacancy diffuser for GaAs and computational models have suggested that negatively charged vacancies have lower formation energies in higher n-type background concentrations which could explain the significant Si diffusion observed.[13–18] It is possible that a vacancy mechanism is also significant contributor to silicon diffusion in InGaAs.

The possibility of transient-enhanced diffusion (TED) was explored by measuring the diffusivity as a function of annealing time for anneals at 550–750 °C as shown in Fig. 4. The Fickian component of diffusivity decreased by less than a factor of 4 from the maximum diffusivity for a given annealing temperature, while the concentration-dependent component of diffusion decreased by less than a factor of 3. A modest decrease in diffusivity as a function of annealing time suggests that TED is not a major contributor to the observed Si diffusion.

This work presents significant concentration-dependent diffusion of implanted Si in $In_{0.53}Ga_{0.47}As$. A major factor that differs from prior studies are the peak concentrations of Si achieved, which are much higher than the solid solubility limit of $\sim 3 \times 10^{19}\,cm^{-3}$. Also, it was determined that TED was not a contributing factor of dopant redistribution.

The authors would like to thank the Semiconductor Research Cooperation for supporting this work. They would also like to thank Applied Materials for providing the implants and InGaAs substrates as well as Evans Analytical group for SIMS. Also, thanks to Aaron Lilak at Intel and Nicholas Vito for helpful discussions.

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