Modeling B Uphill Diffusion in the Presence of Ge

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Abstract

Several models for B diffusion in $Si_{1-x}Ge_x$ have been proposed [1, 2]. In order to help discriminate between the models, an experiment was performed. Preamorphized Si wafers were implanted with varying doses of Ge, followed by a B implant. Samples were annealed at several temperatures. Ge implanted samples showed an increase in the B profile peak magnitude with anneal time, as well as its shift towards the surface. Control samples, receiving two Si implants, showed the expected enhanced B diffusion and none of the uphill diffusion behavior. Simulations accounting for the formation of GeB complex show qualitative fit to the measured profiles.

1. Introduction

Boron is the dopant of choice for p-type silicon, its behavior determines the parasitic resistances and capacitances in source/drain regions of a p-type metal-oxide-semiconductor field effect transistor (pMOSFET). The interest of the modeling community is directed at the anomalous diffusion, namely transient enhanced diffusion (TED) [3], deactivation through formation of boron-interstitial clusters (BICs) [3, 4], as well as reduced diffusion in $Si_{1-x}Ge_x$ [5, 1]. Investigation of Moriya et al. [1] showed reduction of B diffusion with increasing Ge content in MBE grown $Si_{1-x}Ge_x$ layers. In modeling those effects, Ge presence was treated as a perturbation of the bandgap. The simulation provided profiles close to the experiment using the bandgap narrowing, ΔE_G, similar to other measurement methods. Lever et al. [2] suggested a model of Ge reacting with B, forming immobile GeB complex. The idea of a GeB complex was based on the possibility of microscopic strain relaxation. Based on experimental evidence of Kuo et al. [6], macroscopic strain influence was considered negligible. The model [2] included the clustering reaction, as well as bandgap narrowing due to Ge presence, successfully modeling diffusion of B through regions with 3% and 10% Ge. The GeB complex was also observed microscopically, via β-NMR [7], in $Si_{1-x}Ge_x$ with x ranging from 1.7% to 7.5%. In subsequent work [8], *ab-initio* simulations of $Si_{1-x}Ge_x$, suggest that GeB complex formation relaxes the lattice constant of $Si_{1-x}Ge_x$ towards resembling that of pure Si. Macroscopically observed Ge effect on activation energy of B diffusion at concentrations ~5e20 cm^{-3} [9] further supports the notion of clustering.

2. Experimental

Two float-zone (FZ) n-type Si <100> wafers, resistivity 70-130 Ωcm, were preamorphized by a silicon implant at liquid nitrogen temperatures with dose of 1.0e15 cm^{-2} and the energy of 100keV. Following the preamorphization implant (PAI), one wafer was implanted with a Ge dose of 4e15 cm^{-2} at 30keV. The control wafer received another Si implant with 1e15 cm^{-2} at 30 keV, ensuring amorphization in the near surface region. Finally, both wafers received the same B implant, with dose of 2e14 cm^{-2} at 10 keV. Anneals were performed in inert N_2 ambient. Anneals shorter than 15 minutes were performed in an RTA, using 125 ^oC/s ramp up rate.

3. Discussion and modeling

The deep silicon PAI guarantees subsequent implants are completely contained within the existing 0.2μm thick amorphous layer (Fig1), not influencing its depth. By the same virtue, end of range (EOR) damage does not vary with respect to B or Ge implant dose. Silicon PAI was performed at liquid nitrogen temperature to ensure the backflow of interstitials from the EOR damage towards the surface[10, 11], as opposed to formation of a loop layer capturing interstitials diffusing to the surface [12]. TED resulting from self-interstitial clusters in EOR would increase the difference between Si only implanted samples and Ge implanted samples, in case of a clustering reaction. If that is the case, one would be able to discriminate it against the Ge dose. A clustering peak could not be the consequence of BICs, as previous experiments showed BICs do not form in preamorphized, and then regrown layers [11]. The time dependence of B profile evolution at 800^{o}C is shown in figure 2. The increase in the profile peak magnitude, as well as lack of the profile portion below the peak of as-implanted profile indicate the uphill diffusion.

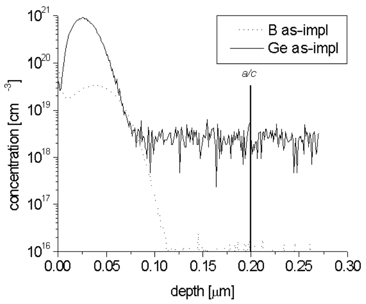

Figure 1. Profiles of B and Ge in as-implanted material, with a/c interface position.

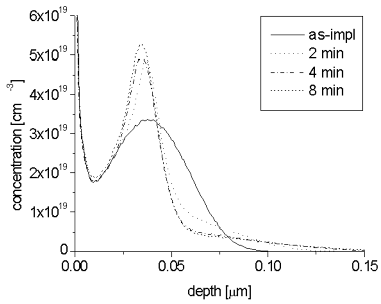

Figure 2. Boron profiles of Ge implanted wafer show distinct uphill diffusion during annealing at 800^{o}C. Uphill diffusion ceases by the TED's end.

As EOR releases all its interstitials during the transient of TED, these interstitials provide the diffusion enhancement. In this case, the diffusing specie (BI pair) seems to cluster in the proximity of Ge profile. To investigate the phenomena further, anneals were performed at 700^{o}C. The profile evolution of Ge implanted samples, and Si only implanted (control) samples, are shown in figures 3 and 4, respectively.

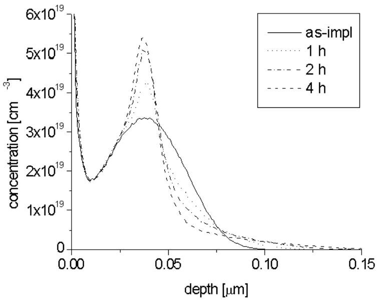

Figure 3. Boron profiles of Ge implanted wafer during annealing at 700°C.

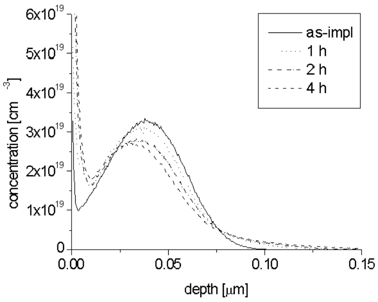

Figure 4. Boron profiles of control wafer (no Ge implant) during 700°C anneal. TED is observed, but no uphill diffusion.

The Ge implanted sample shows uphill diffusion similar to the 800°C anneal. The control sample exhibits TED with diffusion enhancement on the order of several hundreds, but none of the uphill diffusion behavior seen in the Ge implanted sample. The distinction between figures 3 and 4 confirms the phenomena to be qualitatively different from that reported in Duffy et al. [13], as the interstitial gradient should be very similar in both Ge implanted and control samples.

a)

b)

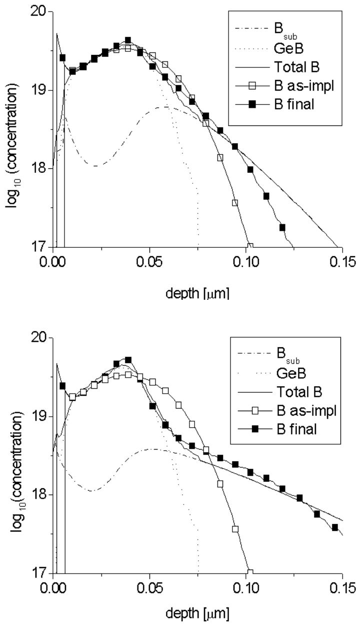

Figure 5. Simulated profiles during 700°C anneal at: a) 1 hour, and b) 4 hours. Measured profiles (SIMS) are also denoted by symbols.

a)

b)

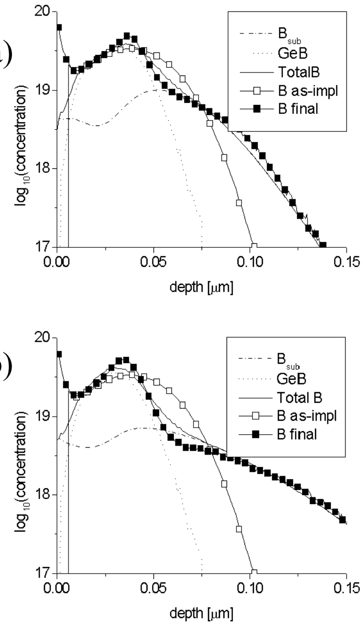

Figure 6. Simulated profiles during 800°C anneal at: a) 2 minutes, and b) 8 minutes. Measured profiles (SIMS) are also denoted by symbols.

The model used to describe the phenomena is a Florida Object Oriented Process Simulator (FLOOPS) implementation of B diffusion model. Based on *ab-initio* energetics of Windl et al. [14], BI pair is the only B mobile species. The trapping of B at Ge sites is governed by a clustering reaction (1), a slight modification of previously described model [2].

$$BI + Ge \leftrightarrow GeB + Int \tag{1}$$

Bandgap narrowing [15] due to Ge presence is taken into account while solving Poisson equation. Simulation results for 700 and 800^{o}C are shown in figures 5 and 6, respectively. The lines represent simulated profiles, while lines with symbols represent measured SIMS profiles. One can notice that the increase in the B profile peak is due to GeB complex formation. The simulation shows the correct behavior of uphill diffusion, although not capturing the exact increase in the profile peak.

4. Conclusion

The observed phenomenon of B uphill diffusion is dependent on Ge presence. Its time dependence is characterized for temperatures of 700 and 800^{o}C. Using models available in the literature, the phenomenon is modeled achieving a qualitative fit to experimentally measured profiles.

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