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Probing the Behaviors of Point Defects in Silicon and Germanium Using Isotope Superlattices

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In order to probe the fundamental behaviors of point defects in silicon and germanium, we studied the self-diffusion using isotope superlattices. In ion-implanted germanium, vacancies are in thermal equilibrium and transient enhanced diffusion is not present under the experimental conditions employed in this study. In contrast, silicon self-interstitials are supersaturated in ion-implanted silicon and the self-interstitial concentration is going down to the thermal equilibrium value toward the surface.

Introduction

Fabrication of the next generation CMOS devices requires fundamental understanding of the behaviors of point defects in silicon (Si) and germanium (Ge) that are characteristic of the nano-scale device processing. Because a variety of point defects generated and absorbed at surfaces and extended defects greatly affects the impurity diffusion, it becomes crucial to understand the transient nature of defect diffusion related to the nano-CMOS fabrications. In this study, we studied the self-diffusion in Si and Ge using isotope superlattices (SLs) to probe the fundamental behaviors of point defects. First, we measured Ge self-diffusion using ion-implanted Ge SLs in order to investigate whether transient enhanced diffusion (TED) due to implantation damage does exist or not. Next, Si self-diffusion during TED was investigated using ion-implanted Si SLs. Based on the experimental diffusion profiles, we simulated the time evolution of Si self-interstitials during TED in Si

Ge superlattices

The recent growth in interest in Ge devices has encouraged researchers to revisit fundamental studies of Ge. The need for further studies is illustrated by our limited understanding of the diffusion mechanisms in Ge which is much less advanced than that in Si. For example, while Ge self-diffusion has been known to occur via the vacancy mechanism (1), whether transient enhanced diffusion (TED) due to implantation damage does exist or not, has not been clarified yet. In this study, Ge isotope SLs composed of alternating layers (15 nm) of ^{nat}Ge (^{70}Ge:20.5%, ^{74}Ge:36.5%) and ^{70}Ge (^{70}Ge:96.3%, ^{74}Ge:0.2%) with a ^{nat}Ge cap layer (100 nm) on the top were grown by solid-source molecular beam epitaxy (MBE) (2,3). ^{70}Ge or ^{75}As ions (90 keV, 2×10^{14} cm^{-2}) were implanted into the ^{nat}Ge cap layer of the samples so that the Ge isotope SLs were not

perturbed by the implantation. The samples were annealed at 450–550 ^{o}C in a resistively heated furnace under flowing 99.999% pure Ar. The depth profiles of Ge and As were obtained by secondary ion mass spectrometry (SIMS).

Figure 1 shows the SIMS depth profiles of ^{74}Ge in the Ge SLs implanted with ^{70}Ge and without implantation, followed by annealing at 550 ^{o}C for 2.5 h. The implanted ^{70}Ge profiles were obtained by TRIM calculation (4). Note that the actual interfaces between ^{nat}Ge and ^{74}Ge layers are abrupt and the smearing of the ^{nat}Ge and ^{74}Ge profiles is due to the SIMS artifact (knock-on mixing, *etc.*). As clearly seen in Fig. 1, Ge self-diffusion in the Ge implanted SLs showed no significant difference from that without Ge implantation. In addition, the Ge self-diffusivity to fit the data agreed well with the reported thermal diffusivities of Ge vacancies (1), being independent of annealing times. Moreover, Ge self- and As diffusion in the As implanted SLs was also found to be in thermal equilibrium with no time dependence because the thermal Ge self- and As diffusivities (5,6) well reproduced the SIMS profiles in the simulation that takes into account doubly negatively charged vacancies (V^{2-}) (3). This indicates that TED was not present under the experimental conditions employed in this study. The absence of TED is quite different from the diffusion in implanted Si, where the diffusion is significantly enhanced by implantation-induced damages and shows the time dependence, as will be directly shown in the next section.

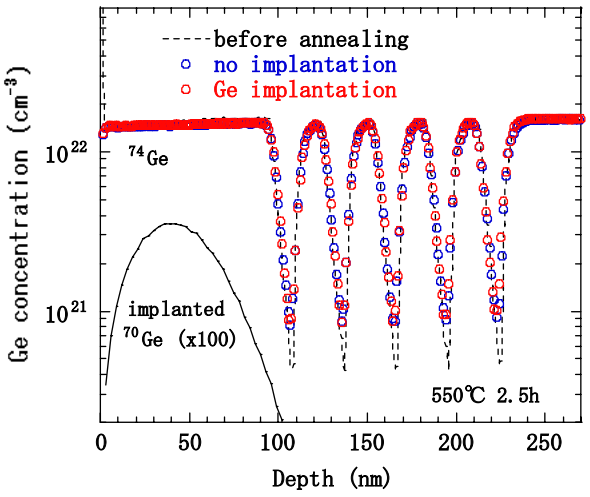

Figure 1. SIMS depth profiles of ^{74}Ge in the ^{nat}Ge/^{70}Ge isotope SLs implanted with ^{70}Ge at 90 keV, 2x10^{14} cm^{-2} and without implantation after annealing at 550 °C for 2.5 h. The broken line represents the profile before annealing. The implanted ^{70}Ge profile is calculated by TRIM.

Si superlattices

For precise modeling of impurity diffusion in Si during the formation of shallow junctions, thorough understanding of the diffusion mechanisms involving TED is required. Regarding TED, {311} self-interstitial clusters produced by ion implantation and annealing are the sources of supersaturated Si self-interstitials, which enhance impurity diffusion (7). In order to develop a diffusion model toward more precise process simulators, investigations of the behavior of the Si self-interstitials are required, especially in the initial diffusion process, where TED occurs and the diffusion takes place

under non-equilibrium point defect conditions. In this study, Si isotope SLs composed of alternating layers of ^{nat}Si(10 nm) and ^{28}Si(10 nm) were grown by MBE (8,9). The SL samples were implanted with ^{28}Si ions (30 keV, 3x10^{14} cm^{-2}) and were annealed at 800–850 ^{o}C under flowing Ar.

Figure 2 shows the depth profiles of ^{30}Si in the ^{28}Si-implanted Si isotope SLs, followed by annealing at 850 ^{o}C for 1 and 4 h. Here, ^{nat}Si layers have a natural abundance with 3.1% of ^{30}Si, whereas ^{28}Si layers are depleted of ^{30}Si. The implanted ^{28}Si profile (not shown) has a peak concentration of ~6x10^{19} cm^{-3} at ~45 nm. With such an implantation condition, the periodic depth profile of ^{30}Si is almost unperturbed after the implantation. Note that the actual interfaces between ^{nat}Si and ^{28}Si layers are abrupt and the smearing of the profiles is due to the SIMS artifact. In Fig. 2, Si self-diffusion much faster than that of the equilibrium diffusion was observed within the first 1 h of annealing, confirming TED in Si. In addition, the enhancement of Si self-diffusion is observed at the deeper region compared with that of the diffusion near the surface. This directly shows that the concentration of Si self-interstitials supersaturated by {311} self-interstitial clusters is going down to the thermal equilibrium values toward the surface (10). Although such a gradient of Si self-interstitials toward the surface was reported by the measurement using B marker layers (11), the present work reports the direct observation of the enhanced Si self-diffusion using Si isotope SLs.

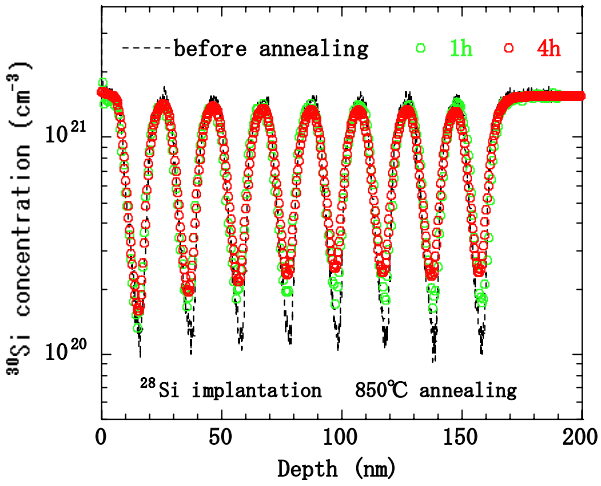

Figure 2. SIMS depth profiles of ^{30}Si in the ^{nat}Si/^{28}Si isotope SLs implanted with ^{28}Si at 30 keV, 3x10^{14} cm^{-2} after annealing at 850 °C for 1 and 4 h. The broken line represents the profile before annealing.

We simulated the Si isotope profiles in Fig. 2 based on our diffusion model (10) and investigated the time evolution of Si self-interstitials during this process. The simulated supersaturations of Si self-interstitials (the ratio between the concentration of Si self-interstitials and that at thermal equilibrium) during 0–1 h annealing are drawn in Fig. 3. The Si self-interstitials are severely supersaturated (~10^{4}) at the initial stage (1 s) with a flat profile in the bulk, whereas the value is going down to the equilibrium concentration toward the surface. At 60 s, the concentration is decreased to 10^{-3} compared with a value at 1 s. As annealing time increases, the concentration approaches the equilibrium value. As shown in Fig. 2, a slower self-diffusion was observed between 1 and 4 h compared with that during 0–1 h, and our simulation shows that the Si self-diffusion is in the thermal equilibrium for longer annealing times.

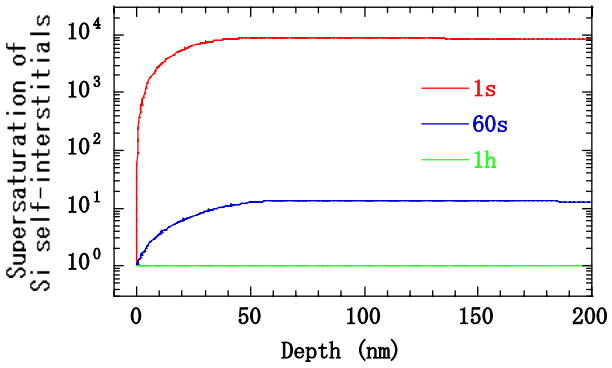

Figure 3. Simulated supersaturations of Si self-interstitials corresponding to Fig. 2.

Conclusions

Diffusion in Ge was found to be in thermal equilibrium and no time dependence was observed for ion-implanted Ge, whose dose would be high enough to induce TED in Si. In contrast, Si self-interstitials are supersaturated in ion-implanted Si and the Si self-interstitial concentration is going down to the thermal equilibrium value toward the surface.

Acknowledgments

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