Phosphorus Redistribution Caused by Electrical Deactivation of Phosphorus at Low Temperatures

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Abstract—Electrical deactivation of phosphorus was investigated using silicon-on-insulator (SOI) wafers with uniform phosphorus profiles prepared by ion implantation and annealing at high temperatures. Evident depletion of phosphorus was observed in the bulk region of the active silicon layer when electrical deactivation of phosphorus occurred at low temperatures. Such phenomenon was due to uphill diffusion of phosphorus toward the surface. Retrograde profiles of excess interstitials generated during deactivation were proposed to explain the redistribution of phosphorus.

Keywords—phosphorus; deactivation; diffusion; interstitial; silicon-on-insulator

I. INTRODUCTION

The size of metal-oxide-semiconductor field effect transistors (MOSFETs) has been scaled down to improve the operation speed of integrated circuits. MOSFETs with a fin structure or ultrathin silicon body were developed to suppress short-channel effects. For such devices, the cross-sectional area along the channel is small. There are less dopants in the source/drain extension region. This may degrade the switching speed of transistors because of the high resistance of the extension regions. Therefore, annealing at high temperatures was preferred to promote dopant activation. On the other hand, dopant diffusion needs to be controlled for small transistors. Consequently, laser annealing was adopted for dopant activation [1]. Among n-type dopants, phosphorous can provide doping layers with low resistivity. However, significant phosphorus deactivation was observed during low-temperature annealing following laser activation [2]. Serious deactivation of phosphorus occurred at temperatures around 600 °C, which was much lower than that for boron. However, both boron and phosphorus diffuse via interstitials. Reference [2] also demonstrated tail diffusion of phosphorus and enhanced diffusion of embedded boron atoms during deactivation. This implies that deactivation is also related to reactions of point defects. In this paper, deactivation of phosphorus was further investigated using uniform phosphorus doping in SOI samples. Evident redistribution of phosphorus near the surface region was observed during phosphorus deactivation.

II. EXPERIMENTAL

Figure 1 shows the experimental procedure. (100)-oriented p-type were used in this study. The SOI wafers have an active silicon layer with a thickness of 200 nm. After a screen oxide with a thickness of 15 nm was grown at the surface, phosphorus at different doses was implanted into the silicon layer. Furnace annealing (FA) at 1100 °C for 2 hr was performed to remove implantation damage and obtain uniform doping. When FA was performed, cool down took a long time. This may produce some dopant deactivation. Therefore, an additional rapid thermal annealing (RTA) at 1100 °C for 1 min was applied to improve dopant activation. Then phosphorus deactivation was induced by FA at low temperatures. Hall measurement was conducted to analyze the dose of active phosphorus atoms. Samples were cycled between FA and Hall measurement. Redistribution of phosphorus was monitored by secondary ion mass spectrometry (SIMS).

![Fig. 1. Experimental procedure for this study.](image-url)
III. RESULTS AND DISCUSSION

Figure 2 shows sheet resistance during FA at 600 °C after initial activation at 1100 °C. The sheet resistance decreased with the increase of phosphorus implantation doses. When the implantation dose increased to 5x10^16 cm^-2, there was no further reduction in sheet resistance. This indicates that phosphorus activation already reached its limitation. Most of the phosphorus atoms in samples implanted at a dose of 5x10^16 cm^-2 were not electrically active. During annealing at 600 °C, there was almost no change in the sheet resistance of the samples implanted at a dose of 1.5x10^15 cm^-2. This implies that there was no evident out diffusion of phosphorus during long-time annealing. This also indicates no reactions between phosphorus atoms. However, the sheet resistance of samples with phosphorus implantation doses higher than 5x10^15 cm^-2 increased with time. Clearly, this indicates formation of phosphorus complexes due to interactions between phosphorus atoms. Interestingly, the sheet resistance of samples implanted at 5x10^16 cm^-2 was even higher than that of samples implanted at a dose of 5x10^15 cm^-2 after deactivation.

Figure 3 shows the Hall mobility for samples during annealing at 600 °C. The samples with phosphorus implantation at a dose of 1.5x10^15 cm^-2 did not show evident change in Hall mobility. However, all the other samples showed increasing Hall mobility with time. The increase of Hall mobility was associated with phosphorus deactivation. When the concentration of active dopants decreased, the effect of ionized impurity scattering on carrier mobility also decreased. This explains why the samples implanted by a dose of 5x10^15 cm^-2 demonstrated a mobility higher than that of samples implanted at 1x10^16 cm^-2. It turns out that these samples with different implantation doses had similar sheet resistance. The lowest Hall mobility was demonstrated by the samples with an implantation dose of 5x10^16 cm^-2. The low mobility is believed to be due to inactive phosphorus because most of the phosphorus atoms in the samples were not active. Since phosphorus activation in these samples cannot be improved, the low mobility caused the sheet resistance higher than that in samples with lower implantation doses.

Based on above discussion, the deactivation behaviors of samples with implantation doses of 5x10^15 and 1x10^16 cm^-2 were focused in our study. Figure 4 plots the active dose of phosphorus during deactivation annealing at 600 and 750 °C for samples with phosphorus implantation at a dose of 5x10^15 cm^-2. The initial active dose after RTA at 1100 °C is less than the dose of phosphorus implantation. This is possibly due to phosphorus segregation at the interface between silicon and oxide. Interface segregation can cause significant dose loss of phosphorus in silicon [3]. The active dose of phosphorus continuously decay after annealing at 600 °C. Almost 40 % of the active dose was lost during annealing for 640 min. For deactivation at 750 °C, rapid decay of active dose occurred at the beginning of annealing. This indicates that the interaction between phosphorus atoms became faster when annealing temperature increased. However, the deactivation saturated after annealing for long times. The saturation of deactivation implies balance of formation and dissolution of phosphorus complexes. At 600 °C, formation of complexes dominated phosphorus deactivation. The dissolution rate of complexes increased at 750 °C such that saturation of deactivation was observed.
Figure 5 presents phosphorus deactivation for samples implanted with phosphorus at a dose of 1x10^{16} cm^{-2}. A small portion of phosphorus was not active. However, the inactive dopants seem not to have evident impact on dopant deactivation, according to the deactivation behavior observed in samples implanted at a dose of 5x10^{15} cm^{-2}. A extremely fast deactivation occurred in 20 min during annealing at 600°C. Then the deactivation of phosphorus continued with a slow deactivation rate. The deactivation curve governed by the slow deactivation rate is almost parallel to that for samples with phosphorus implantation at a dose of 5x10^{15} cm^{-2}. This implies a slow mechanism for deactivation during long-time annealing. The deactivation at the beginning of annealing is caused by another fast mechanism, possibly due to reactions with high-concentration phosphorus. It is not surprised that a similar fast deactivation was observed in the curve for samples annealed at 750°C. Saturation of deactivation was also shown during annealing 750°C. However, the saturation level for samples implanted at a dose of 1x10^{16} cm^{-2} is higher than that for samples implanted at a dose of 5x10^{15} cm^{-2}. This indicates that the saturation of deactivation only represents a steady state, not an equilibrium condition.

The SIMS profiles for samples implanted at a dose of 5x10^{15} cm^{-2} were shown in Fig. 6. The initial phosphorus profile after RTA at 1100 °C is almost uniform except a tiny dip at each boundary of the silicon layer due to interface segregation. Decrease of phosphorus concentration was observed in the bulk region of silicon during deactivation at 600 °C. The percentage loss of phosphorus dose in the bulk region was around 8%. Evident pile-up of phosphorus was observed at the two boundaries. Although quantitative SIMS analysis cannot be applied at the boundaries due to different yields of secondary ions in silicon and oxide layers, the increase of phosphorus signal still indicates some pile-up of phosphorus. For samples annealed at 750 °C, the depleton of phosphorus in the regions nearby silicon boundaries clearly indicates uphill diffusion toward the interface. The percentage dose loss in the bulk region was about 13%. Because screen oxide was removed for Hall measurement during deactivation, the depletion profile is not totally symmetrical.

Figure 7 shows the SIMS profiles for samples implanted at 1 x 10^{16} cm^{-2}. Phosphorus depletion near the two silicon boundaries were observed at 600 °C. The profile became more asymmetrical at 750 °C. There was also more phosphorus signal observed at the front surface. However, the dose of phosphorus lost in the bulk region remained the same level as that in samples implanted at 5x10^{15} cm^{-2}. It seems that the amount of mobile phosphorus species did not increase with the increasing phosphorus concentration. The redistribution of phosphorus at low temperatures implies generation of excess point defects. Because the initial phosphorus profiles in this study were uniform, excess interstitials brought by emitter-push effect can be neglected. Takamura et al. proposed interstitial ejecting during deactivation of phosphorus [2]. Uphill diffusion of phosphorus was reported [4-5] when transient enhanced diffusion was induced by implantation damage. In order to verify the effect of excess interstitials, process simulation was performed using TSUPREM-4 [6]. Uniform profiles of phosphorus and interstitials were placed in an SOI structure. Redistribution of phosphorus and interstitials

Fig. 5. Deactivation of phosphorus for samples implanted by phosphorus at a dose of 1x10^{16} cm^{-2}.

Fig. 6. SIMS profiles of phosphorus for samples with phosphorus implantation at a dose of 5x10^{15} cm^{-2}.

Fig. 7. Phosphorus SIMS profiles for samples implanted by phosphorus at a dose of 1x10^{16} cm^{-2}.
was simulated at 600 °C. Figure 8 shows the simulation results. The excess interstitials produces a retrograde profiles near the surface. The profile resulted in uphill diffusion of phosphorus toward surface and the dose of phosphorus in the bulk region was therefore reduced. For generation of evident uphill diffusion, the level of excess interstitials was about $10^5$ to $10^6$ times larger than the equilibrium concentration of interstitials. This is consistent with the diffusion enhancement extracted from the embedded boron marker layer by Takamura et al. [2].

IV. CONCLUSIONS

In summary, phosphorus deactivation was investigated by uniform phosphorus profiles in SOI wafers. Redistribution of phosphorus profiles was observed during deactivation even though the initial profiles of phosphorus were almost flat. Such phenomenon is attributed to the generation of interstitials during phosphorus deactivation. The retrograde interstitial profile near the surface caused uphill diffusion of phosphorus. Phosphorus uphill diffusion caused pile-up at the surface and reduction of dose in the bulk region.

REFERENCES