Effect of Oxidation Ambient on Phosphorus Diffusion in SOI

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Phosphorus diffusion profiles in bulk and SOI substrates were measured by SIMS, spreading resistance and four point probe methods and the accuracy of the measured profiles was discussed each other. Using the measured phosphorus diffusion profiles, the main diffusion parameters involved in the phosphorus-point defect pair diffusion model were determined.

1. Introduction

SOI (Silicon on Insulator) structure is promising as a substrate for future highly efficient LSIs, because of low parasitic capacitance and easy device isolation. The SOI structure has silicon-silicon dioxide interface, then diffusion profiles in the SOI are presumed to be different from those in the bulk, since the interface will act as a sink or source for point defects.

The most interesting n-type dopant species in silicon LSI technology is phosphorus because phosphorus which diffusion profiles show plateau shape in the 10^{20} cm^{-3} region, kink shape in the 10^{19} cm^{-3} region and tail shape in the region below 10^{18} cm^{-3} [1].

The purpose of this work is to clarify the phosphorus diffusion model in SOI structures and to obtain the accurate simulation parameters. To obtain the experimental data, phosphorus was diffused at 900 °C to bulk and two kinds of SOI with different active layer thickness in nitrogen and oxygen ambients. The profiles were measured by spreading resistance (SR) method, SIMS and four point probe method with anodic oxidation. Then, the measured profiles were compared with simulated ones using the simulator TSUPREM-4 in which several main diffusion parameters were changed and best-fitted parameter set was determined [2,3].

2. Experimental

2.1 Substrate & Diffusion Condition

Substrates used are p-type (100) bulk silicon and two kinds of bonding SOI substrates with 2.2 μm and 10μm active layer thicknesses. Resistivity of these substrates was in the range of 5 to 20 Ω-cm. Phosphorus predeposition step was carried out using the spin-on-glass source at 900 °C for 20 min and 370 min in nitrogen ambient. For 20 min predeposition, after removal of the glass source, drive-in step was done at 900 °C for 350 min in nitrogen or oxygen ambients. These sample preparations are summarized in Table I.

Table I Experimental condition

Substrates			
bulk p-type (100) 5-10Ωcm	bulk n-type (100) 5-10Ωcm	SOI(10μm) p-type (100) 4-6Ωcm	SOI(2.2μm) p-type (100) 14-22Ωcm

Diffusion conditions	
900°C	370 min predeposition
	20 min predeposition + 350 min drive-in in N_2
	20 min predeposition + 350 min drive-in in O_2

Measurement of profile		
SIMS	SR method	Four point probe method*

(*Sheet resistivity measurement and anodic oxidation are repeated)

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2.2 Measurement of Diffusion Profile

Phosphorus diffusion profiles were measured by SR method (SSM-150ESS), SIMS (CAMECA-4f) and four point probe method in which sheet resistivity measurement and anodic oxidation were repeated.

The phosphorus predeposition profiles measured by the three kinds of methods are shown in Fig. 1 where the diffusion was done at 900 °C for 370 min for bulk silicon. The profiles are somewhat different each other. In the high concentration region above 10^{20} cm^{-3}, i.e., near the surface, the SIMS profile shows the highest concentration which will be caused by the presence of non-active phosphorus atoms or the increase of secondary ion counts due to surface natural oxide, while the profile by SR method shows significantly lower concentration, compared with other two methods. In the middle concentration region from 10^{19} cm^{-3} to 10^{18} cm^{-3}, the three kinds of profiles are very much similar each other. Below 10^{18} cm^{-3}, i.e., near the pn junction, the profile by SR method shows the shallowest one, compared with those by SIMS and four point probe methods.

From these results, it is concluded that the profile in the higher concentration region than 10^{19} cm^{-3} should be determined by four point probe and SIMS methods; in the region from 10^{19} cm^{-3} to 10^{18} cm^{-3} the above three methods show almost the same profile; in the region below 10^{18} cm^{-3} the SIMS profile is most reliable.

2.3 SR Measurement in Low Concentration Region near pn Junction

The SR method is the most convenient to measure profiles, i.e., easier and cheaper than other two methods. So, if the correct profile is obtained by SR method, it has an great advantage over other methods. In the present work, we studied the cause of shallower profile measured by SR method in the region near pn junction.

To study the effect of pn junction on SR measurement, we compared the phosphorus diffusion profiles for p-type and n-type substrates, as shown in Fig. 2. The diffusion was done at 900 °C for 20 min and 370 min. For n-type substrate, the SR value increases monotonously with depth and reaches to constant value corresponding to the substrate, while for p-type substrate, the SR value has a peak (which is assumed to be depletion layer edge) and reaches to the constant value beyond it. Furthermore, in the p-type substrate, the peak value for long time (370 min) diffusion is higher than the constant value, while the peak value for short time (20 min) diffusion is lower than the constant value. From Fig. 2, we can assume the depletion layer (DL) edge, the depths equal to p-type and n-type substrate concentrations and estimated metallurgical junction (MJ) depth. Fig. 3 shows such four kinds of depth. For long time diffusion, i.e., deep diffusion, these depths converges the same values, and for short diffusion time, i.e., shallow

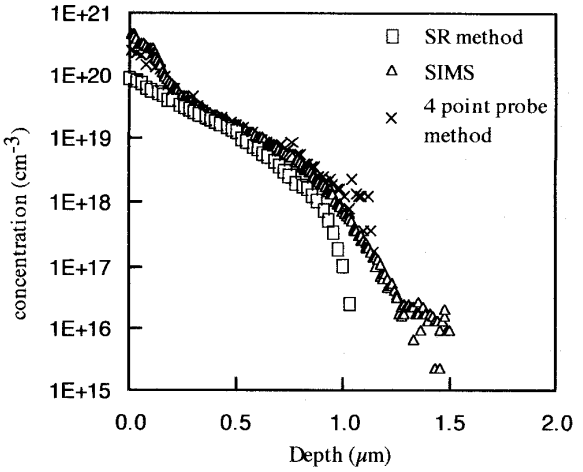

Fig. 1 Phosphorus diffusion profiles measured by three kinds of method

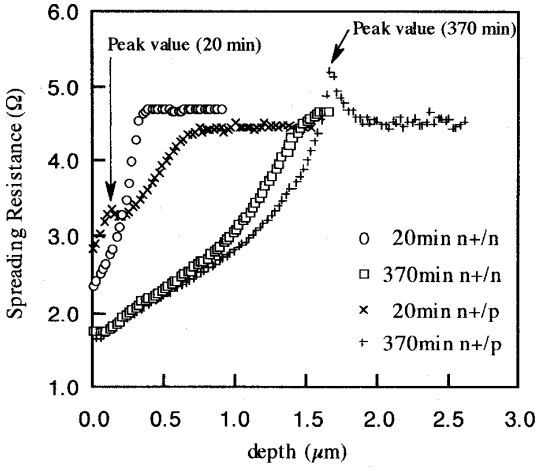

Fig. 2 SR measurement profiles with/without pn junction

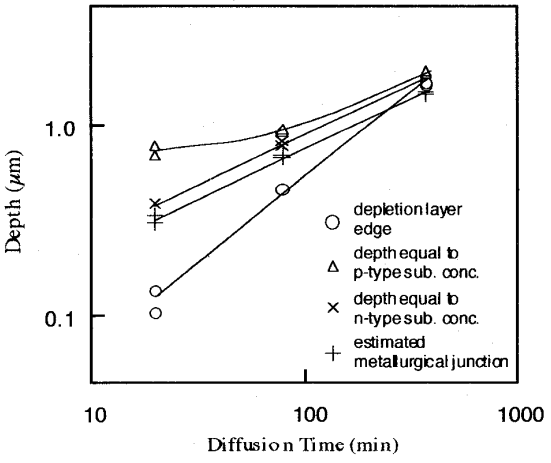

Fig. 3 Typical depths vs diffusion time in SR depth profile.

diffusion, the DL edge differs significantly from the estimated MJ depth.

From these experiments, it is confirmed that the correct profile in the low concentration near pn junction by the SR method can be obtained by using the same type substrate, i.e., n-type substrate for phosphorus diffusion.

3. Simulation Procedure

We simulated diffusion profiles using the popular simulator on the market, TSUPREM-4 which has three kinds of diffusion models. Of them, we used "pd.full" model which involves the diffusion mechanism due to phosphorus-point defect pair and also represents behaviors under non-equilibrium condition. The charge states of point defects, i.e., interstitial and vacancy, are assumed to be neutral, negative and double negative.

The fitting procedure of measured profiles to simulated ones is carried out by changing the main three diffusion parameters as shown schematically in Figs. 4 and 5. For the first, the ratio of interstitial mechanism to total (interstitial and vacancy mechanism), f_{PI} is determined to fit the plateau and kink shape above 10^{19} cm^{-3} region in the measured profile. Second, the diffusion coefficient of interstitial (which is assumed to be equal to vacancy diffusion coefficient), DI is determined tentatively to fit the measured profiles for 370 min predeposition, especially, to fit the tail region below 10^{18} cm^{-3}. Thirdly, the recombination velocity of interstitial at silicon-silicon dioxide interface, K_{surf} is determined to fit the profiles for diffusion in oxygen ambient and also in two kinds of SOI substrates. The second step and third step mentioned above are repeated to obtain the best fitting.

4. Results & Discussion

The parameter, f_{PI} controls the high concentration region, i.e., the plateau and kink shapes; With larger f_{PI}, the plateau becomes smaller and above 0.95 of f_{PI}, the plateau disappears, while with smaller f_{PI}, the kink becomes smaller, and below 0.75 of f_{PI}, the kink disappears as shown in Fig. 6. The best fit value of f_{PI} for the present experiments is 0.85.

Next, D_I governs the total diffusion depth, in other words, the tail region in the profile, as shown in Fig. 7. If larger D_I is chosen, then diffusion depth become shallower. This is explained as follows; larger D_I causes the interstitial move faster into deeper region, then phosphorus atoms can't make pairs with interstitial and as a result, phosphorus diffuses more slowly. The best-fit of D_I is $1.83*10^{-4}\exp(-1.58/kT)$.

Since K_{surf} relates to both oxidation surface and buried oxide interface, the diffusion profile in oxygen ambient changes largely with the value of K_{surf}. Fig. 8 shows an experimental profile and three simulated profiles with different K_{surf} values. From Fig. 8, we can obtain the K_{surf} value of $4.2*10^{-6}\exp(1.75/kT)$ for best-fit one.

4.Conclusion

To obtain reliable experimental diffusion profiles, we should use different measurement method: For higher concentration region than 10^{19} cm^{-3}, four point probe method with anodic oxidation and SIMS gives reliable profiles; For middle concentration range from 10^{19} to 10^{18} cm^{-3}, SR, SIMS and four point probe methods gives almost the same profiles; For lower concentration near junction, SIMS method gives the most reliable profile, and SR method gives also the good profile when the same type substrate is used.

The three main phosphorus diffusion parameters, f_{PI}, D_I and K_{surf} in the simulator TSUPREM-4 were determined to best-fit the measured profile at 900°C and shown in Table II.

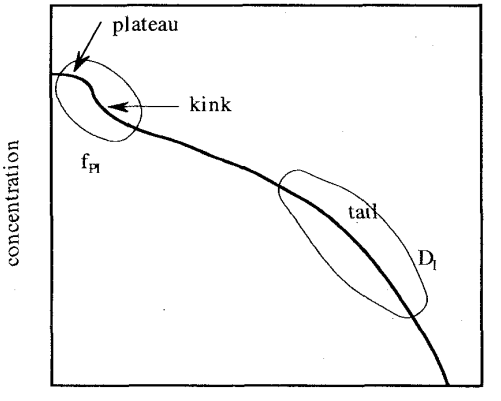

Fig. 4 Effect of simulation parameters f_{PI} and D_I on phosphorus profiles

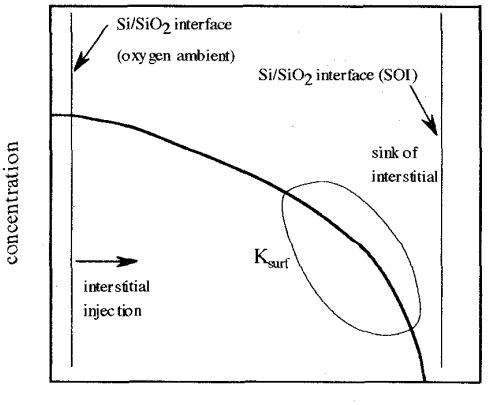

Fig. 5 Effect of simulation parameter Ksurf on profile

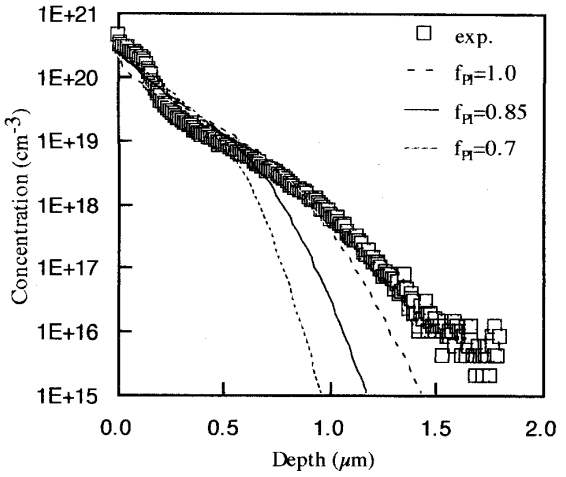

Fig. 6 Comparison of experimental and simulated profiles for parameter fPI values

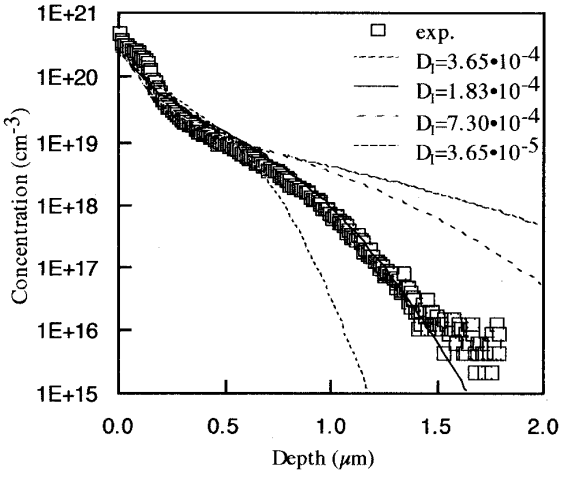

Fig. 7 Comparison of experimental and simulated profiles for parameter DI values

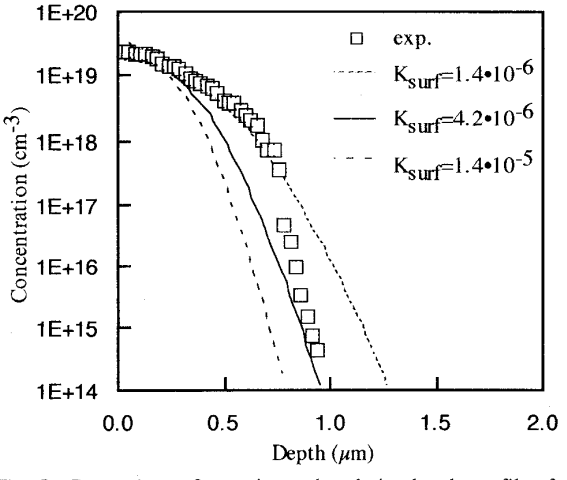

Fig. 8 Comparison of experimental and simulated profiles for parameter Ksurf values

Table II Best-fit values of TSUPREM-4 parameters for bonding SOI

Parameter	(unit)	Value (default)
F_{PI}		0.85 (1.0)
$D_I(=D_V)$	(cm^2/sec)	1.83 • 10-4 exp (-1.58/*k*T) (3.65 • 10-4 exp (-1.58/*k*T))
K_{surf}	(cm/sec)	4.2 • 10-6 exp (1.75/*k*T) (1.4 • 10-6 exp (1.75/*k*T))

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