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Fraction of Interstitialcy Component of Phosphorus and Antimony Diffusion in Silicon

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1. Introduction

It is recognized that dopants in Si such as boron, phosphorus and antimony diffuse via point defects(self-interstitials or vacancies). A fractional interstitial component of dopant diffusion, f_I, is one of key parameter in process simulation. Untill now it has been determined by calculating the point defect concentration which is less reliable. Its value of each dopant varies widely depending on the experimental conditions.

Recently, we found that excess vacancies were introduced in the Si substrate under Si_3N_4 films due to the thermal stress at the interface[1],[2]. That is, Si_3N_4 films can be used as the extrinsic source of vacancies.

In this work, we investigate the diffusion of phosphorus and antimony in Si under Si_3N_4 films at the same time and determine the interstitialcy fraction of these dopants explicitly without calculating point defect concentration.

2. Experimental

The used substrates were p-type (100) FZ-Si with resistivity of 4~6 Ω cm. Phosphorus or antimony ions were implanted through 50 nm thermally grown oxide with doses of $3\times10^{13}/cm^2$ at 100keV. After activation annealing, oxide films were partly removed and Si_3N_4 films were deposited by ECR plasma CVD and two types of area were prepared. The deposited Si_3N_4 films were 200nm thick. One area had a SiO_2/ Si_3N_4 double layered film (ON-area) in which the normal diffusion occurs, and the other had a Si_3N_4 film (N-area) in which vacancy supersaturation is caused (Fig.1). Samples were annealed at 900°C~1100°C for 360min in dry N_2 to diffuse phosphorus or antimony. Phosphorus junction depth and antimony diffusion profiles were measured by staining technique and SIMS, respectively.

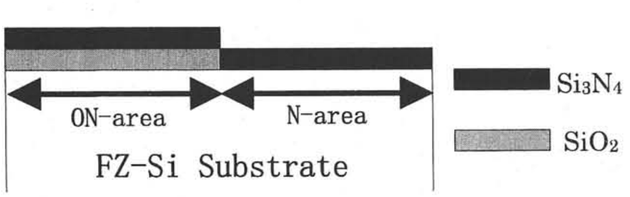

Fig.1: Cross-sectional view of samples

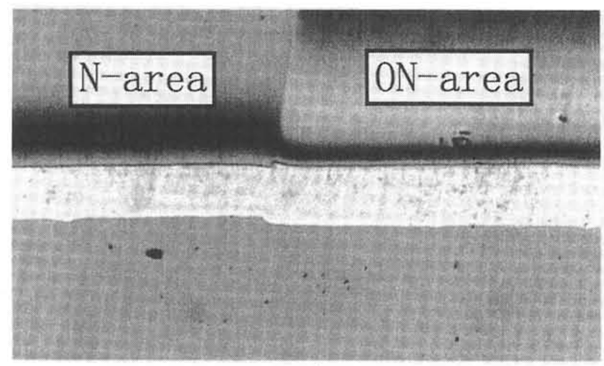

Fig.2: Junction profile of phosphorus annealing at 1000°C for 360min.

3. Results and Discussion

Figure.2 shows the phosphorus junction depths from the sample annealed for 360min in dry N_2 at 1000°C. One notes that the phosphorus diffusion under N-area is retarded as compared to that under ON-area. In contrast to phosphorus, after annealing at 1000°C for 360min as shown in Fig.3, the antimony diffusion in N-area is enhanced. This dendency was also observed in the temperature range from 900 to 1100°C and diffusivities both under N-area and under ON-area, that is D_N and D_{ON} respectively, were determined from the fitting procedure. Figure.4 shows D_N/D_{ON} as a function of the reciprocal of temperature. In Fig.4, D_N/D_{ON} for phosphorus changes from 0.4 to 0.76 and for antimony from 7.24 to 1.18 in the temperature range from 900 to 1100°C and the degree of both retardation of phosphorus diffusion and enhancement of antimony diffusion becomes smaller as the temperature becomes higher.

The relation between dopant diffusivities(D_A) and point defects in Si can be described by

$$\frac{D_A}{D_A^*} = f_I\frac{C_I}{C_I^*} + (1-f_I)\frac{C_V}{C_V^*} \tag{1}$$

where C_I and C_V are the concentration of silicon self-interstitial and vacancy respectively. Asterisk * denotes each thermal equilibrium values and f_I is a fraction of

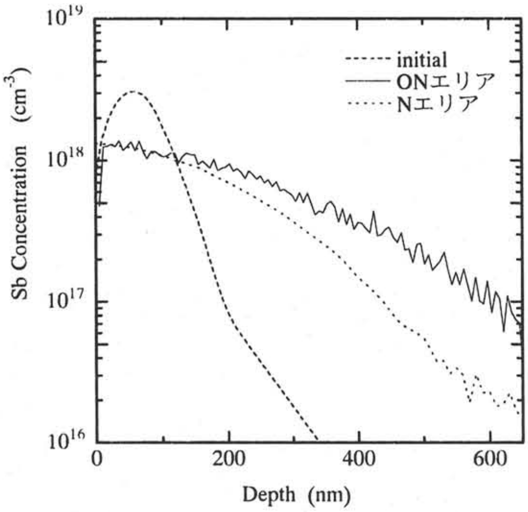

Fig.3: antimony concentration profiles after annealing at 1000°C for 360min.

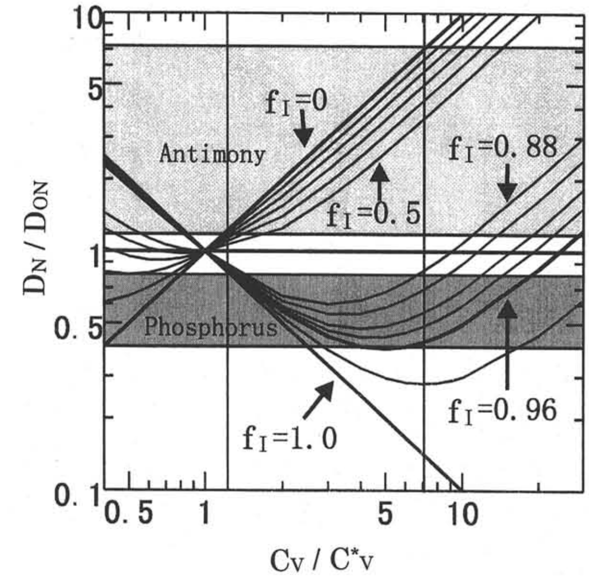

Fig.5: D_N/D_{ON} as a function of C_V/C^*_V

interstitial-related diffusion. D_N/D_{ON} is calculated as a function of C_V/C^*_V from the combination of eq.(1) and the law of mass action, $C_I C_V = C^*_I C^*_V$ and is shown in Fig.5 with a parameter of f_I, which is set every 0.02 from 0.88 to 1.0 and every 0.1 from 0 to 0.5.

Since the effect of Si_3N_4 films on phosphorus and antimony diffusion depends on the diffusion temperature from Fig.4, the supersaturaion rate of vacancy also depends on it. So it is reasonable to consider that 1/T corresponds to C_V/C^*_V. Shaded areas in Fig.5 show the experimental data of D_N/D_{ON} of phosphorus and antimony diffusion. Since diffusion of phosphorus and antimony was performed under same conditions, supersaturated value of vacancy was the same in both diffusion. Therefore the degree of enhancement in antimony and retardation of phosphorus diffusion should be satisfied simultaneously for values of C_V/C^*_V generated at the corresponding diffusion temperatures. Considering the above requirement, values of f_I of both phosphorus and antimony diffusion are determined: f_I=0.96 for phosphorus and f_I=0 for antimony. Thus vacancy component is contributed a little to phosphorus diffusion while vacancy mechanism almost dominates in antimony diffusion as reported previously.

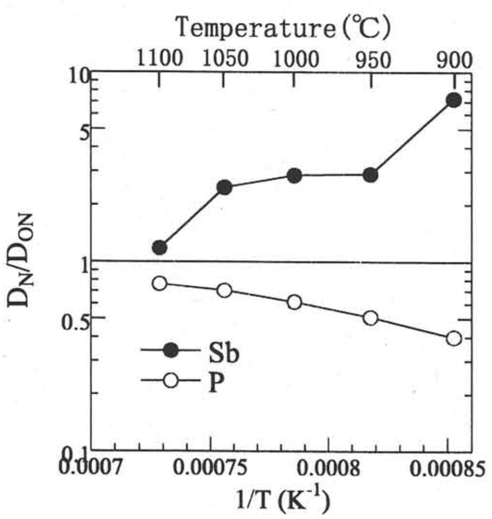

Fig.4: D_N/D_{ON} as a function of annealing temperature.

4. Conclusion

Diffusion of phosphorus and antimony in Si under Si_3N_4 films has been investigated. By observing the degree of the retardation in phosphorus diffusion and the enhancement in antimony diffusion under Si_3N_4 films, it is determined that fraction of interstitialcy component in phosphorus and antimony diffusion appoximately 0.96 and 0, respectively.

Acknowledgments

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