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# Determination of Vacancy Diffusivity in Silicon for Process Simulation

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## Abstract

Vacancy diffusivity has been determined by using the fact that $Si_3N_4$ films deposited on silicon can be used as an extrinsic source of vacancies. Excess vacancies generated at the backside with $Si_3N_4$ films migrate to the boron-implanted region at the top side and its boron diffusion is retarded. Using these data, vacancy diffusivity is determined from the simulation.

## 1. Introduction

Process simulation becomes more important with the shrinkage of the device dimensions in ULSI. Development of numerical method and establishment of physical model are essential for progress of process simulation. The present situation is, however, far from reality, mainly due to the lack of the reliable physical model [1] . Dopant diffusion is known to be one of the key process in ULSI technology and its accurate prediction is essential to device simulators. It has been recognized that dopant diffusion in silicon is mediated by interaction of dopant atoms with both vacancies and self-interstitials [2] . Thus many physical parameters of point defects (vacancy and silicon self-interstitial) are necessary for the simulation of dopant diffusion.

Self-interstitial diffusivity has been extensively studied because oxidation was the extrinsic source of self-interstitials. However, most parameters are still uncertain. Particulary, there are very few data about vacancy diffusivity.

Recently, we investigated the vacancy concentration in boron-diffused region in Si under both $Si_3N_4$ and $SiO_2$ /$Si_3N_4$ films by slow positron beam technique and found that excess vacancies were introduced in the Si substrate under $Si_3N_4$ films due to the thermal stress at the interface [3][4] . That is, $Si_3N_4$ films can be used as the extrinsic source of vacancies.

In this work, we tried to determine vacancy diffusivity based on the simple concept. The method determining vacancy diffusivity is consisting of the following three steps: (1) generation of excess vacancies at the backside with $Si_3N_4$ films, (2) observation of vacancy migration by boron diffusion at the top side, (3) estimation of vacancy diffusivity by the simulation.

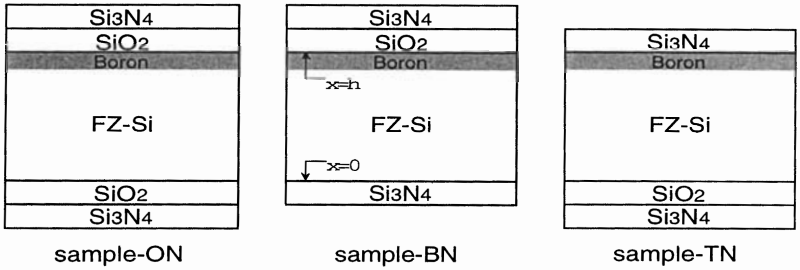

Figure 1: Sample structures.

## 2. Experimental

Based on the above concept, samples having different structures shown in Fig.1 were prepared. Starting materials were p-type FZ (100) Si single crystals with resistivity of 3-5 Ωcm and thickness of 238 μm. First, boron implanted regions were formed at the top side by ion implantation with an energy of 70 keV and a dose of $7.5\times10^{13}\mathrm{cm}^{-2}$ through 50 nm oxide. Samples were annealed at 900°C in $N_2$ for 30 min to restore the damage. For sample-BN, oxide at the backside was removed and for sample-TN, oxide at the top side was etched off. Then stoichiometric $Si_3N_4$ films were deposited by ECR plasma CVD to both sides using $SiH_4$ and $N_2$ gases. The thickness of $Si_3N_4$ was 50 nm. Cross section of the respective sample structures is shown in Fig.1. The sample-ON has a structure with $SiO_2$ /$Si_3N_4$ double layered films at both sides. Boron diffusivity obtained from sample-ON corresponds to the intrinsic diffusivity of boron [5] , which is used as a reference. Using sample-BN, the migration of vacancies from the backside is monitored by the diffusion of boron at the top side. The sample-TN is necessary for the determination of excess vacancy concentration generated under $Si_3N_4$ films, which is used as the boundary condition as described later. Annealing was performed in $N_2$ at 1000°C for 10, 33, 70, 129 h. After etching $SiO_2$ and $Si_3N_4$ films, boron concentration profiles were measured by secondary ion mass spectroscopy (SIMS)(ATOMIKA 6500). The boron diffusivity of Si, $\langle D_B\rangle$, was determined by fitting measured profiles with simulated plofiles obtained by solving Fick's diffusion equation.

## 3. Results and Disscussion

A typical example of boron concentration profiles obtained from respective sample structures by SIMS analysis is shown in Fig.2 after annealing at 1000°C for 129 hr. Boron diffusion in sample-BN is retarded as compared with that of sample-ON. The annealing time dependence of the ratio of boron diffusivity, $\langle D_B\rangle$ to that of sample-ON(intrinsic diffusivity), $D_B^*$ is shown in Fig.3. At 10 h, its ratio is nearly 1. It means that excess vacancies migrating from the backside recombine almost with self-interstitials in the bulk and does not reach the top side. Above 30 h, they reach at the top side and cause the undersaturarion of self-interstitials, that is, retardation of boron diffusion. In sample-TN, boron diffusion is also retarded as shown in Fig.2. The annealing time dependence of $\langle D_B\rangle/D_B^*$ is shown in Fig.3. In sample-TN, retarded diffusion of boron is observed at 10 h and its ratio decreases slightly with the increase of annealing time.

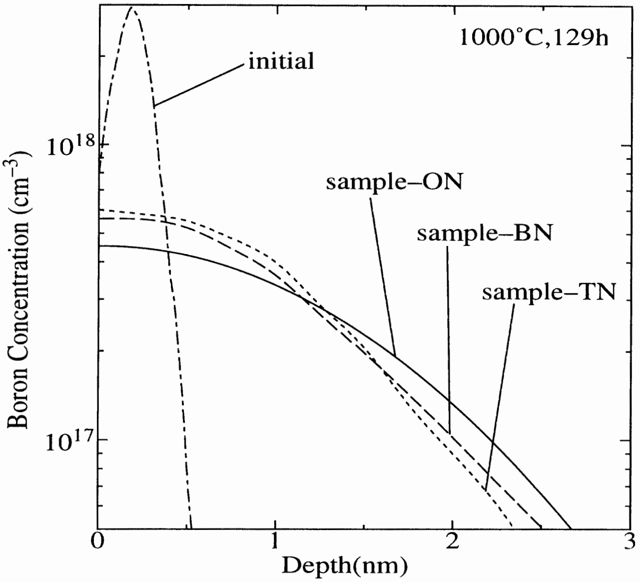

Figure 2: Boron concentration profiles of respective samples.

*Simulation of $D_V$ and $k_V$*

1. Estimation of vacancy concentration at the top side in sample-BN by solving the diffusion equation of vacancy with the appropriate boundary conditions.

$$\frac{\partial C'(x,t)}{\partial t} = D_V \frac{\partial^2 C'(x,t)}{\partial x^2}, \quad (0 < x < h) \tag{1}$$

where $C'(x,t)$ is the normalized vacancy concentration $(= C_V(x,t)/C_V^*)$, $C_V$ and $C_V^*$ are the vacancy concentration and its equilibrium value, respectively, $D_V$ is the vacancy diffusivity, and $h$ is the thickness of the substrate.

Boundary conditions;

$$\textit{at the backside} \quad (x = 0), \quad C'(0,t) = P(t) \tag{2}$$

where $P(t)$ is the excess vacancy concentration generated at the Si/Si$_3$N$_4$ interface and is given from the experimental data of sample-TN.

$$\textit{At the top side} \quad (x = h), \quad D_V \frac{\partial C'}{\partial x}_{x=h} + k_V \left[C'(h,t) - 1\right] = 0 \tag{3}$$

where $k_V$ is the recombination rate of vacancy at Si/SiO$_2$ interface.

2. Determination of vacancy diffusivity and recombination rate by fitting procedure. Boron diffusivity at the top side is estimated from the following equation.

$$\left\langle \frac{D_B}{D_B^*} \right\rangle = f_I \left\langle \frac{C_I}{C_I^*} \right\rangle + (1 - f_I) \left\langle \frac{C_V}{C_V^*} \right\rangle \tag{4}$$

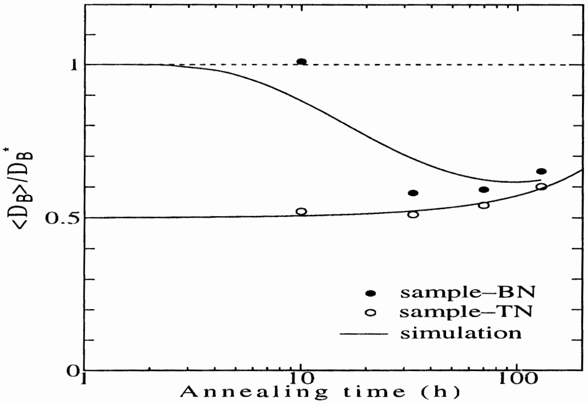

Figure 3: Annealing time dependence of $\langle D_B \rangle / D_B^*$ of sample-BN and sample-TN

where $f_I$ is the fraction of interstitialcy mechanism. When the vacancy concentration is given from the above procedure, boron diffusivity can be caluculated as a function of time.

In the caluculation, we assume $f_I$=1 for boron diffusion. Local equilibrium condition that $C_V C_I = C_V^* C_I^*$ is also assumed. Changing both $D_V$ and $k_V$, fitting the calculated with the experimental data is repeated. Two solid lines in Fig.3 are the simulated results using the values that $D_V = 4.1 \times 10^{-9}\text{cm}^2/\text{s}$ and $k_V = 8.9 \times 10^{-10}\text{cm/s}$ at 1000°C. It is concluded that physical quantities relating vacancy can be determined based on the experimental results.

## 4. Acknowlegement

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