A New Physical Model for Thermal Oxidation of Silicon

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Thermal oxidation of silicon generates silicon self-interstitials, leading to the enhanced diffusion (OED) of phosphorus or boron. This well-known phenomenon, however, have been studied only from the point of anomalous impurity diffusion. In this paper, we propose a new kinetic model which account for the pressure dependence of thermal oxidation as well as the experimental results of impurity diffusion.

During thermal oxidation of silicon, oxygen molecules which diffused toward the Si/SiO_2 interface through the previously formed oxide react with the silicon substrate. Volume expansion accompanied with the reaction causes the generation of self-interstitials. Because of the difference of chemical potential for the silicon atom between the silicon bulk and the oxide, most of the generated excess silicon atoms flow into the bulk oxide and quickly react with the oxygen molecules near the interface as shown in Fig. 1. Surface regrowth process also annihilates self-interstitials at the interface. The flux into the bulk silicon, causing the anomalous impurity diffusion, is negligibly small compared to the other factors as is indicated by the experimental results.[1)]

Under these conditions, the concentration of self-interstitials at the interface is expressed as a function of the oxygen concentration at the interface as shown in Fig. 2.

$$\frac{C_I}{C_I^*} = \frac{\gamma}{\beta} \frac{C_o + \beta}{C_o^{0.5} + \gamma} \tag{1}$$

where C_o denotes the concentration of oxygen molecules at the Si/SiO_2 interface. β and γ are the physical parameters including reaction rate constant at the interface, k_d, and the recombination constant of silicon self-interstitials at the interface, K. C_{oc} is the critical oxygen concentration at which the interstitial concentration becomes its equilibrium value.

Since large number of self-interstitials flow into the oxide, the oxidation rate is expressed as a sum of two oxidation mechanisms: (1) direct reaction at the interface and (2) the oxidation of self-interstitials in the oxide. Using Eq.(1), the observed oxidation rate is given by

$$N \frac{dX}{dt} = k_d C_o + k_d C_o^{0.5} \frac{C_o + \beta}{C_o^{0.5} + \gamma} \tag{2}$$

where first term of the right hand side denotes the direct reaction while the second term the oxidation of self-interstitials in the oxide.

All of the kinetics at the interface described above are schematically illustrated in Fig. 3.

In order to explain both orientation and pressure dependence of thermal oxidation, we assume $k_d^{(111)} > k_d^{(100)}$ and $K^{(111)} >> K^{(100)}$ because there exist much more surface kinks on the (111) plane than the (100) plane. Based on these assumptions, Eq.(2) leads to the pressure dependence of thermal oxidation rate as shown in Fig. 4. Noted that oxidation rate sublinearly depends on the concentration of the oxygen molecules at the interface, oxidation rate of (100) plane is larger than that of (111) plane at low partial pressure, while at high pressure the oxidation rate reversed. These features are exactly the same as the experimental observation.

In summary, we developed a new kinetic model at the Si/SiO_2 interface during oxidation by incorporating the flow of silicon self-interstitials into the oxide, which well explains various phenomena relating to silicon oxidation.

1) K. Taniguchi, Y. Shibata and C. Hamaguchi, *J.Appl.Phys.*65,2723 (1989).

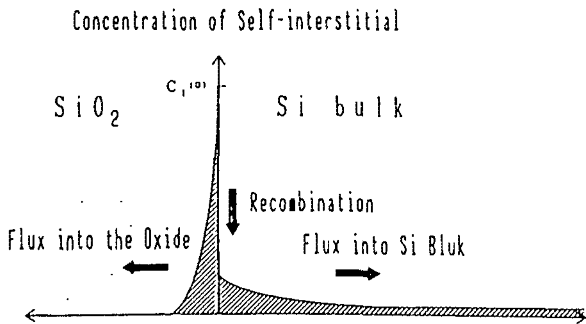

Fig. 1 Schematic representation of the distribution of silicon self-interstitials near the Si/SiO_2 interface.

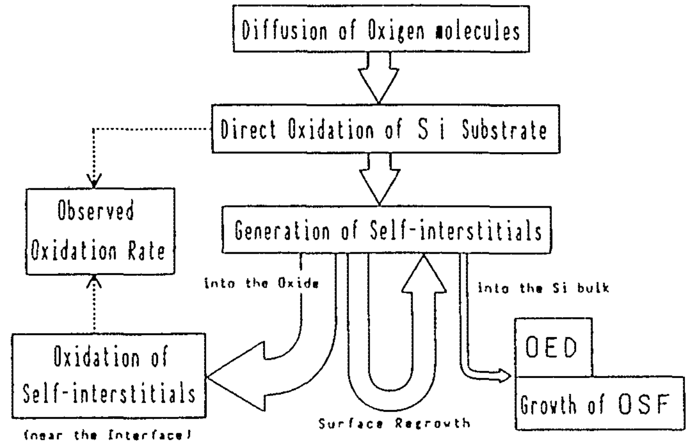

Fig. 3 Schematic diagram of the new physical model.

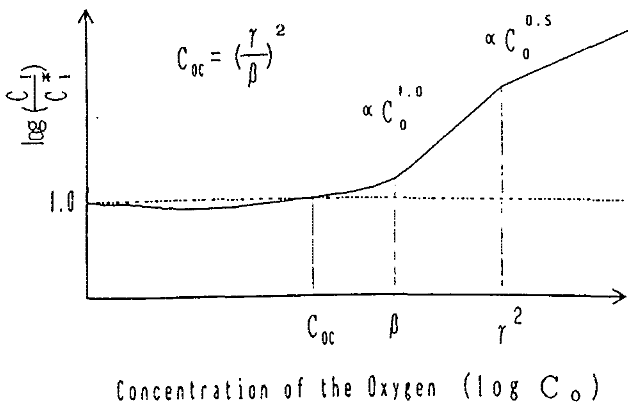

Fig. 2 Normalized concentration of silicon self-interstitials vs the concentration of oxygen molecules at the Si/SiO_2 interface.

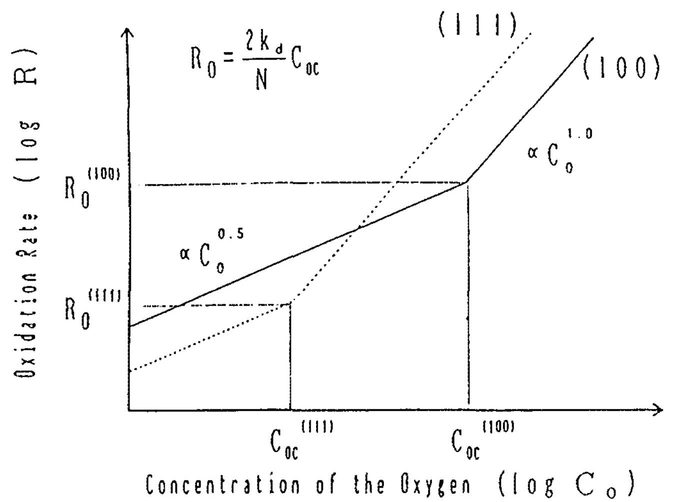

Fig. 4 The relation between oxidation rate and oxygen concentration at the interface. R_o is the critical oxidation rate which gives the equilibrium concentration of silicon self-interstitials.