

Modelling of silicon interstitial surface recombination velocity at non-oxidizing interfaces

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Abstract

In this work we present a model for the surface recombination velocity of silicon interstitials at non oxidizing interfaces. The model takes in to account the experimentally observed diffusion of silicon atoms through an oxide. The influence of the interfacial region in also discussed.

1. Introduction

Point defect interaction at non oxidizing interfaces is of fundamental importance for accurate simulation of thermal processes in silicon. Silicon interstitial recombination at non-oxidizing interfaces has been historically modelled as

$$F_S = \sigma_{\text{eff}} (C_I(t) - C_I^{\text{eq}}) \quad (1)$$

where σ_{eff} is the surface recombination velocity, $C_I(t)$ and C_I^{eq} are the actual and the equilibrium concentration of interstitials at the interface. From the physical point of view this approach indicates that the interface acts as a infinite sink for interstitials. However one would rather expect that the ability of the interface to absorb interstitials is decreasing with time, probably by the filling up of the sites where the atoms can interact [1]. Experimental results obtained from backsurface oxidation-front surface stacking fault grow experiments with silicon membranes [2] indicate that σ_{eff} is a decreasing function of time, and not time independent, as it is usually assumed.

In this work we present a model for the surface recombination velocity of silicon interstitials at non oxidizing interfaces. The model accounts for the diffusion of silicon

atoms through the oxide as well as the influence of the interfacial layer between the silicon and the oxide.

2. The model

In a previous work[3] we have shown that when a silicon interstitial reaches the interface with the oxide it diffuses through it. Although the exact nature of the interaction of interstitials with the oxide is not known, we face two possibilities: either silicon atoms segregate at the interface, or they react with it to form SiO molecules. Subsequently silicon atoms or SiO molecules diffuse in the oxide. It is obvious that correct modelling of the surface recombination velocity must take into account such behaviour.

We assume that silicon interstitial segregate at the silicon-oxide interface and then they diffuse in the oxide. If m is the segregation coefficient for silicon interstitials at the interface, we can express the interstitial flux at the interface as

$$F_s = \sigma_o \left(C_I^{Si} - \frac{C_I^{ox}(t)}{m} \right) \quad (2)$$

where C_I^{Si} , C_I^{ox} are the concentrations at the interface in silicon and in the oxide respectively and σ_o is the surface reaction constant. Neglecting recombination of interstitials at the interface and assuming that interstitials diffuse in the oxide we can solve for the interstitial concentration in the oxide. For convenience we assume that interstitial concentration in silicon near the interface has a constant value and that the oxide has infinite thickness. Equating (1) and (2) and after some mathematical treatment, we find the time dependence of surface recombination velocity,

$$\sigma_{eff} = \sigma_o \exp\left(\frac{t}{t_o}\right) \operatorname{erfc}\left(\sqrt{\frac{t}{t_o}}\right), \quad t_o = \frac{m^2 D}{\sigma_o^2} \quad (3)$$

Fig 1 shows the time dependence of σ_{eff} . From this figure we see that surface recombination velocity remains constant for small values of t/t_o , and gradually decreases with time, according to a t^{-5} law. This is in agreement with the experiments with silicon membranes[2] for the silicon oxide interface for both small and large times. We note that such a time dependence can explain experimental data over a wide range of temperatures and times which predict either constant or time dependent recombination velocity. Similar time dependence is obtained if one assumes formation of SiO at the interface and diffusion in the oxide.

This above analytical model of the surface recombination velocity can be implemented in a process simulator that actually utilises eq.1, with minor code modifications. Besides that one notes that there is only one additional parameter that must be fitted properly.

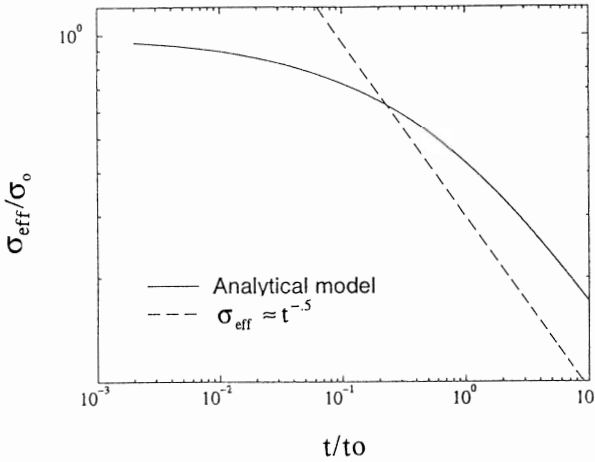


Figure 1: Time dependence of the surface recombination velocity (solid line). We note that σ_{eff} is constant for small values of t/t_0 and gradually decreases with time. The dash line shows a $t^{-0.5}$ dependence

However the silicon-silicon dioxide interface is much more complicated than an ideal plane that imposes boundary conditions. Experimental observations shows that there exist a buffer layer of some finite thickness, between the silicon and the oxide. The physical properties of this layer, eg width, density, stoichiometry, stress, are strongly dependent on the oxidation process as well as any other thermal treatment that takes place. The interaction of silicon atoms with this interfacial layer must have a strong influence on the surface recombination velocity.

Although the exact nature of the interaction is not known, one could assume that there exist some sites inside this layer which act as sinks or traps for silicon atoms. Assume that there exist only one type of trap. Each trap is occupied by 0 or 1 particle. Let Θ be the fraction of traps that are occupied. The diffusion equation inside the interfacial layer is modified to account for the existence of traps.

If we assume that the trapping and detrapping follows a first order kinetic with rate constants k_1 and k_2 respectively then the time evolution of traps is governed by

$$\frac{d\Theta}{dt} = k_1 C_i^{\text{ox}} (1 - \Theta) - k_2 \Theta \quad (4)$$

where C_i^{ox} is the concentration of free silicon atoms in the interfacial region.

However since the problem is more complicated we can obtain only numerical solutions for the silicon / interfacial region / silicon dioxide system. Following the same procedure as above we can calculate σ_{eff} with the presence of traps. A typical result is shown in Fig.2 in comparison with the simple case discussed previously. The influence of the traps

will be more pronounced when the flux of silicon atoms into the traps is larger compared to the diffusion in the oxide. The time dependence of surface recombination velocity in this case becomes more complicated and is dependent on the trap parameters, which are determined by the properties of the interface. However, even in this case eq. 3 could provide a fairly good approximation.

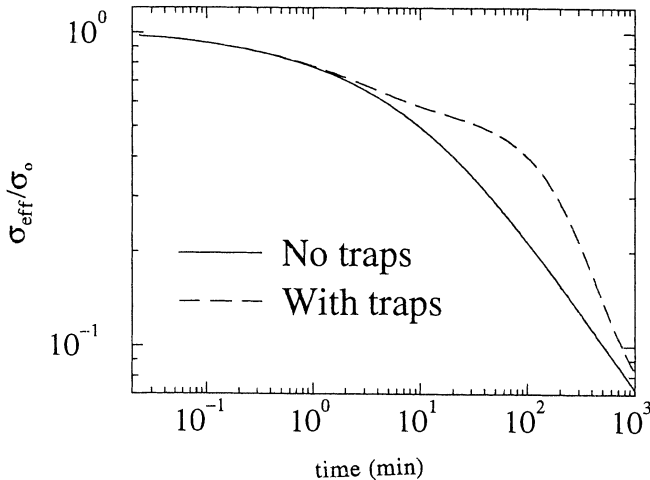


Figure 2: Surface recombination velocity as a function of time with and without traps.

The above analysis is applicable to interfaces of silicon with other materials, eg. silicon nitride. Since silicon atoms have low diffusivity in the nitride, the recombination kinetics will be strongly dependent on the interfacial layer properties. In such cases the surface recombination velocity could fall faster with time, depending on the trap parameters. A $t^{-1.2}$ dependence has been observed for this case [2].

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