Modeling of NBTI Degradation for SiON pMOSFET

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Abstract

For SiO_2 pMOSFETs, the reaction diffusion model is well used to describe the NBTI degradation theoretically and the Ogawa model for hole trap generation is known exper imentally. However, there is not a good model of NBTI degradation for SiON devices. In this paper, we propose a nitrogen dependent hole trap generation model by extending these two models and present the NBTI degradation model for SiON pMOSFETs.

1 Introduction

SiON films have been used as gate insulators for scaled MOSFETs since the beginning of the 1980s [1] and it is well known that nitrogen atoms in SiON reduce boron diffusion from poly Si gate to channel region for pMOSFETs. Threshold voltage shift for SiON pMOSFET under NBTI (negative bias temperature instability) stress is worse than that for pure SiO_2 pMOSFET. Therefore, it is important to clarify the NBTI mechanism and to develop a reliable model of NBTI degradation. The reaction diffusion (RD) model has been proposed by Jeppson *et al.* [2], and applied to investigate the NBTI mechanism for pure SiO_2 devices [3]. However, the NBTI degradation for SiON devices is not explained by the RD model. The purpose of this paper is to develop a novel model to simulate the NBTI degradation for SiON pMOSFETs.

2 Reaction-Diffusion Model

In this section, we briefly review the RD model. The fundamental assumption in the RD model is that the depassivation of hydrogen passivated Si (SiH) bonds at Si/SiO_2 interface during NBTI stress generates hole (h^+) traps at the interface as follows:

$$\mathrm{SiH} + \mathrm{h}^+ \longleftrightarrow (\mathrm{Sih})^+ + \mathrm{H}, \tag{1}$$

where $(\mathrm{Sih})^+$ is interface trap. And the reaction equation is written as

$$\frac{\partial S_{\mathrm{it}}}{\partial t} = k_{\mathrm{f}}(S_0 - S_{\mathrm{it}})p - k_{\mathrm{r}} S_{\mathrm{it}} C_{\mathrm{H}}(0,t), \quad k_{\mathrm{eq}} = k_{\mathrm{f}}/k_{\mathrm{r}}, \tag{2}$$

where k_{f} (k_{r}) is forward (reverse) reaction rate constant of interface trap, k_{eq} equilibrium reaction rate, S_{it} interface trap density, C_{H} hydrogen concentration, S_0 ($= 10^{15}\ \mathrm{cm}^{-2}$ [5]) initial SiH density, t time, and p hole concentration.

In the conventional RD model, k_{eq} is determined so as to reproduce the time depen dence of NBTI degradation, assuming that the diffusivities of H in SiO_2 and poly Si are identical. Fig. 1 depicts typical simulation results, and shows it is difficult to obtain reasonable simulation results for both stress period and relaxation period [8].

3 Effect of H Diffusion on NBTI Degradation

In order to reproduce V_{th} shift in the whole time, we investigated the effect of H diffusion in each region based on [6]. The values of H diffusivity in SiO_2 and poly Si have been experimentally obtained [9, 10] (Fig. 2). Fig. 3 shows the reasonable agreement of simulation result with the experimental V_{th} shift in both periods. Due to smaller diffusivity in the poly Si than that in SiO_2, the poly Si layer acts as a hydrogen reservoir, which results in the quick V_{th} recovery observed in the relaxation period in Fig. 3.
Next, we consider interface trap density S_{it} at stress time t. In Fig. 4, we show hy drogen concentration C_{H} after 1000 s stress time. Since H diffusion to the Si sub strate is negligible, S_{it} corresponds to the total number of hydrogen atoms in SiO_2 and poly Si regions ($S_{\mathrm{it}}(t) \equiv \int_0^\infty C_{\mathrm{H}}(x,t)\mathrm{d}x$). As shown in Fig. 4, we now introduce characteristic diffusion length L_{H}, where trapezoidal area coincides with $S_{\mathrm{it}}(t)$, namely $S_{\mathrm{it}}(t) = (t_{\mathrm{ox}} + L_{\mathrm{H}})C_{\mathrm{H}}(x = 0,t)/2$. Fig. 5 shows the time dependence of L_{H}. Since this figure indicates that L_{H} is approximately proportional to $\sqrt{t}$ in diffusion limited reaction, we write $L_{\mathrm{H}} = \alpha\sqrt{t}$, where α is a parameter. We can see that the gap of L_{H} in the initial phase gives rise to quick V_{th} degradation and recovery. In Fig. 6, we show the extracted values of α and find that α has Arrhenius temperature dependence $\alpha(T) = \alpha_0 \exp(-E_\alpha/k_{\mathrm{B}}T)$. Assuming the equilibrium reaction of Eq. (1) and using $k_{\mathrm{eq}} = k_0 \exp(-E_{\mathrm{k}}/k_{\mathrm{B}}T)$, $S_0 \gg S_{\mathrm{it}}$ and $t_{\mathrm{ox}} \ll L_{\mathrm{H}}$, we obtain the following expression:

$$S_{\mathrm{it}} = \sqrt{k_0 p S_0 \alpha_0/2}\, e^{-(E_{\mathrm{k}}+E_\alpha)/2k_{\mathrm{B}}T}\, t^{1/4}. \quad (3)$$

4 Extended RD Model for SiON pMOSFET

In this section, we newly propose an extended RD model to simulate NBTI degrada tion of SiON gate pMOSFETs. We basically derive the dependence of interfacial trap density on the nitrogen concentration at SiON/Si interface by making use of the Ogawa model [4]. Ogawa *et al.* [4] have empirically derived the following interface trap density in diffusion limited reaction for pure SiO_2 pMOSFET:

$$S_{\mathrm{it}} = \beta E_{\mathrm{ox}}^{3/2} t^{1/4} \exp(-E_{\mathrm{A}}/k_{\mathrm{B}}T)/t_{\mathrm{ox}}, \quad (4)$$

where E_{ox} is electric field in oxide, E_{A} an activation energy, and t_{ox} oxide thickness. Since the nitrogen concentration C_{N} in SiON gate MOSFET is generally 10 atomic% at most, it is considered that the interfacial hole trap at SiON/Si interface gives rise to the dominant effect on the NBTI degradation [11]. Therefore, only the effect of interfacial hole trap is taken into account in the following discussion.
In order to extend the Ogawa model to SiON gate, we adopt C_{N} dependence on β and E_{A} in Eq. (4). Tan *et al.* [12] showed that E_{A} is a function of C_{N} and can be written as

$$E_{\mathrm{A}} = 0.213 - 0.016 C_{\mathrm{N}} \equiv \varepsilon_{\mathrm{A}} + \varepsilon_{\mathrm{N}} C_{\mathrm{N}}. \quad (5)$$

In addition, we derive the coefficient β to reproduce the experimental results [12] for several interfacial nitrogen concentrations. Fig. 7 shows the extracted results. We now introduce the following formulation to express relation between β and C_{N}:

$$\beta(C_{\mathrm{N}}) = \beta_0 (a C_{\mathrm{N}}^b + 1)^{-1}, \quad (6)$$

where a and b are fitting parameters.
Next, we consider the nitrogen dependence in the RD model Eq. (3). By comparison of activation energies in Eq. (3) and Eq. (4), we can naturally obtain the relation $E_{\mathrm{k}} + E_\alpha =$

$2E_A$. By using Eq. (5), the dependence of C_N on E_k is expressed as $E_k = (2\varepsilon_A - E_\alpha) + 2\varepsilon_N C_N$. Since β in Eq. (4) depends on C_N as shown in Eq. (6), it is natural to adopt C_N dependence on the initial trap density S_0. Thus, we obtain the following relation:

$$S_0(C_N) = S_0(C_N = 0) \times (aC_N^b + 1)^{-2}. \quad (7)$$

We apply the extended RD model mentioned above to the simulation of NBTI degradation for several kinds of SiON gate MOSFETs. Fig. 8 shows reasonable agreement of simulation results with experimental ones.

5 Conclusion

We proposed a nitrogen dependent trap model that enables simulation of the NBTI degradation for several kinds of SiON gate MOSFETs. Firstly, we simply formulated the interface trap density for SiO_2 pMOSFET. Secondly, we derived nitrogen dependence of the equilibrium reaction rate of interface trap and activation energy of the equilibrium reaction rate by relating the RD model to the Ogawa model for SiON pMOSFET. As a result, we were able to simulate threshold voltage shift for SiON pMOSFET.

References

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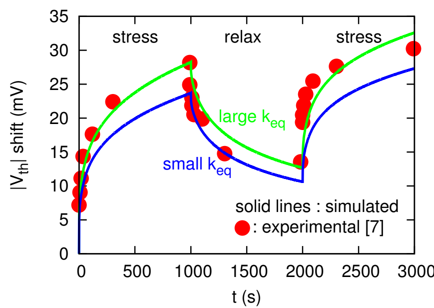

Figure 1: Threshold voltage shift for SiO_2 device as a function of time by making use of the conventional RD model at V_g(stress)$= -2.7$V, V_g(relax)$=$ 0V, $T = 100°$C, $t_{ox} = 1.3$nm.

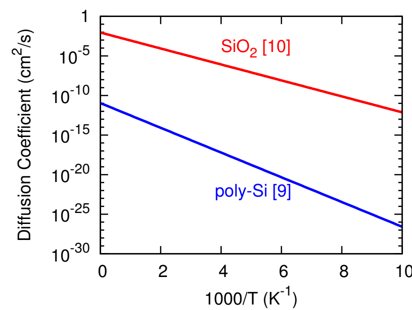

Figure 2: Diffusion coefficient of hydrogen in SiO_2 and in poly Si.

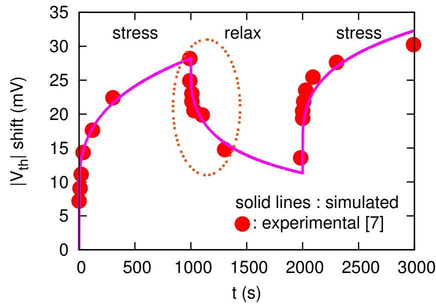

Figure 3: Threshold voltage shift for SiO_2 device as a function of time by making use of the model considering material dependence of hydrogen diffusion coefficient.

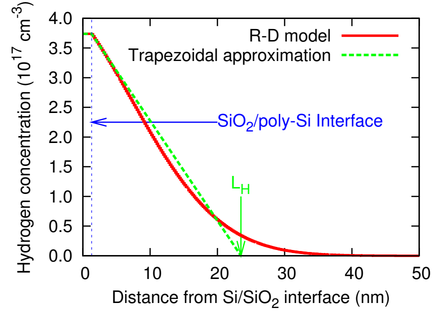

Figure 4: Hydrogen distribution by trapezoidal approximation based on the RD model after 1000 s stress.

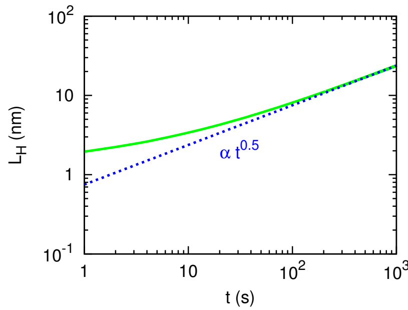

Figure 5: The diffusion length L_H derived from trapezoidal approximation based on the RD model and that from root approximation $\left(\alpha\sqrt{t}\right)$.

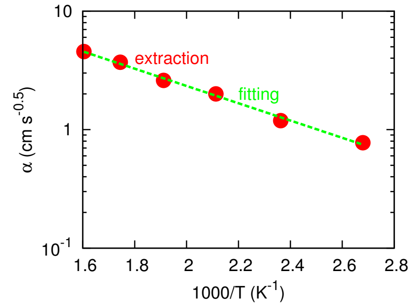

Figure 6: Arrhenius plot of α for several aging temperatures.

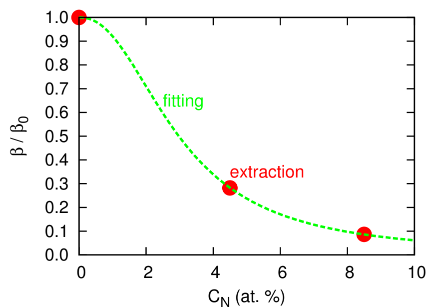

Figure 7: The coefficient of interface trap density as a function of interfacial nitrogen concentration for SiON device at $V_g = -2.2$V, $T = 125°$C, $t_{ox} = 1.8$nm.

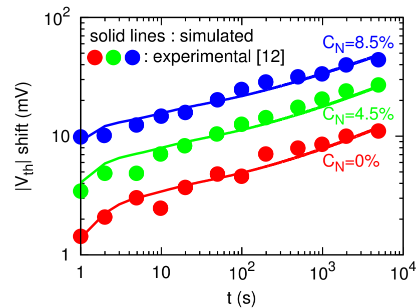

Figure 8: Threshold voltage shift for SiON device as a function of NBTI stress time for several interfacial nitrogen concentrations.