

# Transport-reaction model for interface state build-up at the Si-SiO<sub>2</sub> interface

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## Abstract

The MOS interface state build-up process was simulated for a 1D MOS structure within a framework of reaction-transport model. The identified kinetics is summarized as simple power laws. The transport-limited mode of half power of the stress time has emerged universally with regardless of the charge state of transported species.

## 1 Introduction

Oxide reliability has been an issue since the advent of MOSFETs. Several reaction-transport models have been reported dealing with a 1D MOS problem ( Fig. 1 ) [3, 5, 4]. Their results look somewhat contradictory, as highlighted in Figs 3 and 4. Particularly, the nature of the transport-limited mode is inconclusive. In experiment, on the other hand, Doyle *et al.* identified a universal 0.5 power law of the stressing time or the amount of injected charge[2]. This situation has motivated us to streamline theoretical understanding. Exploring comparison with measurement is beyond the scope of this work.

## 2 Simulated Problem

Interface state(IFS) build-up was simulated within a framework of the surface reaction ( interface state generation and passivation ) and transport phenomena of hydrogen-related species. The rate equation for the surface reaction and the transport equation for the hydrogen-related species were numerically solved with an aid of a partial differential equation solver PROMIS[1]. For simplicity, we have stood back on the simplest situation, a MOS structure as a one dimensional(1D) problem, as illustrated in Figs. 1 and 2.

## 3 Results

### 3.1 IFS kinetics—neutral species involved

Simulation has revealed that the interface state(IFS) build-up process obeys a set of power laws of the stressing time, as shown in Fig. 5. In the course of stressing in Fig. 5, the identified power laws are  $t^1$  (reaction limited),  $t^0$  (quasi-equilibrium),  $t^{1/4}$  ( diffusion limited

mode which fits in Jeppson's solution), and  $t^{1/2}$  ( another diffusion-limited mode ). They fall into two groups; a transport-sensitive mode and a transport-*insensitive* one. The latter two modes of  $t^{1/4}$  and  $t^{1/2}$  are  $D_H$  (diffusivity of the diffusing species in the oxide)-sensitive, as shown in Fig. 6. The  $t^{1/2}$  mode is also  $T_{ox}$  ( oxide thickness )-sensitive. The  $t^{1/4}$  mode does not reveal a  $T_{ox}$  dependence, as shown in Fig. 7. As for neutral diffusing species, power laws are readily summarized in Table 1, most of which can be confirmed also through analytical solution owing to the simplicity of the 1D problem.

### 3.2 IFS kinetics —charged species involved

When charged species are transported, the presence of oxide electric field ( $E_{ox}$ ) creates an asymmetry in IFS kinetics, as shown in Figs. 8–10. When  $E_{ox}$  is repulsive (“+Vg” case in Fig. 8), IFS build-up slows down. When  $E_{ox}$  is attractive (“-Vg” case in Fig. 9), the process is accelerated, with its  $t^{1/2}$  relation unchanged. The  $t^{1/2}$  mode is  $E_{ox}$ -sensitive and branches off at an earlier period as  $E_{ox}$  becomes strong. In the  $t^{1/2}$  mode, IFS concentration was found to be proportional to  $E_{ox}^{1/2}$  (Fig. 10), in contrast to Ogawa[5].

The  $E_{ox}^{1/2}$  dependence was derived also from analytical solution, as summarized in Fig. 11, which supports our numerical simulation and disproves Ogawa's asymptotic solution. Note that the  $E_{ox}$ ,  $T_{ox}$ , and  $D_H$  dependence on IFS is built in the transport coefficient  $A_I^{1/2}$ . The  $E_{ox}^{1/2}$  dependence occurs in the strong  $E_{ox}$  limit. In this limit, an explicit  $T_{ox}$  dependence vanishes. In the opposite limit of weak  $E_{ox}$ , our analytical solution reduces to that for neutral species, which agrees with Hu's solution[3].

### 3.3 Lifetime—sublinearity leverage

Lifetime  $\tau$ , the time which it takes for IFS to reach a threshold, is leveraged by the sub-linear power of time. In the transport-limited mode, the threshold IFS concentration is proportional to  $E_{ox}^{1/2}\tau^{1/2}$ . Solving back this relation with respect to  $\tau$ , the lifetime becomes  $\tau \propto E_{ox}^{-1}$ . When  $E_{ox}$  decreases by a factor of 1/10, IFS build-up slows down by a factor of  $\sqrt{10}$ , but the lifetime increases by a factor of 10. Seeking a less stringent stressing condition, hence, deserves its efforts.

## 4 Conclusion

We applied the reaction-transport model to a 1D MOS structure. The obtained IFS kinetics can be summarized as simple power laws. The transport-limit mode of  $t^{1/2}$  was elaborated using numerical and analytical solutions. Irrespective of neutral or charged species, the transport-limited mode of  $t^{1/2}$  universally occurs. It shows the  $E_{ox}^{1/2}$  dependence for charged species.

## References

- [1] G. Hobler, P. Pichler, and K. Wimmer, “PROMIS 1.5,” Technische Universität Wien, 1989.

- [2] B. S. Doyle, K. R. Mistry, and J. Farichelli, "Examination of the time power law dependencies in hot carrier stressing of n-MOS transistors," *IEEE Electron Device Letters*, vol. 18, pp. 51-53, February 1997.
- [3] C. Hu, S. C. Tam, F.-C. Hsu, P.-K. Ko, T.-Y. Chan, and K. W. Terrill, "Hot-electron-induced MOSFET Degradation—model, monitor, and improvement," *IEEE Trans. Electron Devices*, vol. ED-32, pp. 375-385, February 1985.
- [4] K. O. Jeppson, and C. M. Svensson, "Negative bias stress of MOS devices at high electric fields and degradation of MNOS devices," *J. Appl. Phys.*, vol. 48, pp. 2004-2014, May 1977.
- [5] S. Ogawa, and N. Shiono, "Generalized diffusion-reaction model for the low-field charge-buildup instability at the Si-SiO<sub>2</sub> interface," *Phys. Rev.*, B7, pp. 4218-4230, February 1995.

Table 1: Power law for IFS build-up with neutral diffusing species involved. Exponents for various quantities are listed for "Reaction limited", "Equilibrium", and "Diffusion limited (two types)" modes. In the "2nd diffusion-limited mode," for example,  $N_{IFS}$  is proportional to  $t^{1/2}$ ,  $T_{ox}^{-1/2}$ ,  $(k_G/k_R)^{1/2}$ ,  $D_H^{1/2}$ ,  $C_{SH,0}^{1/2}$ . †denotes  $N_{IFS}$  is proportional only to  $k_G$  rather than the ratio.

Mode	Time t	Oxide thickness $T_{ox}$	Rate constant ratio ( $k_G/k_R$ )	Diffusivity $D_H$	Initial Si-H conc. $C_{SH}$
Reaction limited	1	0	†	0	1
Eqlib.	0	0	1/2	0	1/2
1st diff. limited	+1/4	0	1/2	+1/4	1/2
2nd diff. limited	+1/2	-1/2	1/2	+1/2	1/2

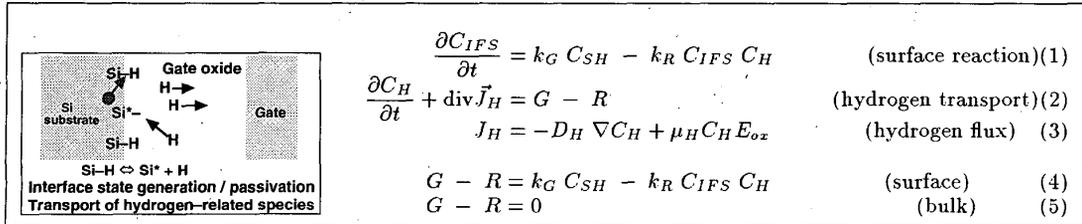


Figure 1: Simulated problem.

<p><math>C_H</math>: concentration of hydrogen species</p> <p><math>C_{IFS}</math>: Interface state concentration</p> <p><math>N_{IFS}</math>: Interface state areal density, <math>N_{IFS} \sim L_R C_{IFS}</math> Assumption: <math>L_R \sim 1\text{nm}</math>(reaction region), <math>C_{IFS}(x) \sim \text{constant for } x \text{ within } L_R</math></p> <p><math>C_{SH}</math>: SiH (IFS precursor) concentration, <math>C_{SH,0}</math>: initial <math>C_{SH}</math></p> <p><math>J_H</math>: hydrogen flux areal density</p> <p><math>D_H</math>: diffusivity for hydrogen species in oxide</p> <p><math>\mu_H</math>: mobility of hydrogen species in oxide, connected with <math>D_H</math> by Einstein relation</p> <p><math>T_{ox}</math>: oxide thickness</p> <p><math>E_{ox}</math>: electric field across the oxide (oxide field)</p> <p><math>k_G, k_R</math>: surface reaction rate constants for IFS generation and passivation (constant in this work)</p> <p><math>k_G</math> includes hot carrier flux.</p>
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Figure 2: Notations.

C. Hu[2]	Jeppson[3]	Ogawa[4]	This work
$N_{IFS}(t) \propto t^{1/2}$	$N_{IFS}(t) \propto t^{1/4}$	$N_{IFS}(t) \propto t^{1/4}, t^{1/2}$	$N_{IFS}(t) \propto t^{1/4}, t^{1/2}$
diffusion limit	diffusion limit	transport limit	transport limit
finite $T_{ox}$ (sink b.c.)	infinite $T_{ox}$	infinite $T_{ox}$	finite $T_{ox}$ (sink b.c.)
neutral	neutral	neutral	neutral
analytical	analytical	ion analytical (asymptotic)	ion numerical

t: stressing time; sink b.c. = sink boundary condition at ox/gate boundary

Figure 3: Previous works and this work.

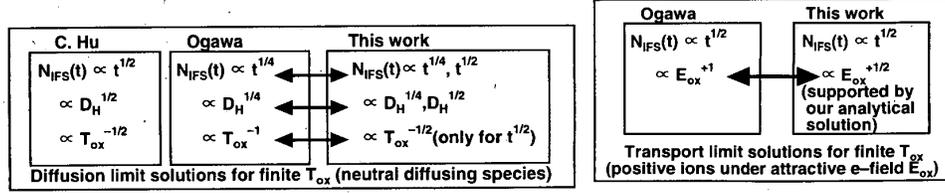


Figure 4: Major differences among works.

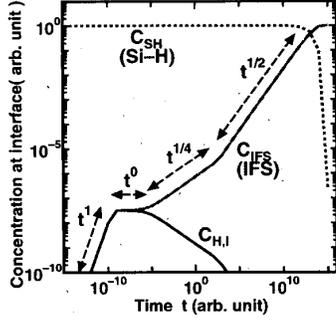


Figure 5: Kinetics for involved species.

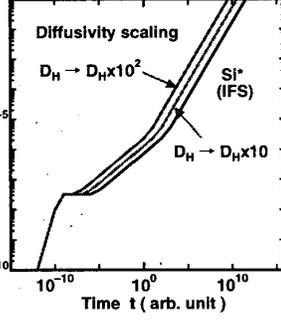


Figure 6: The effects of  $D_H$  on IFS kinetics.

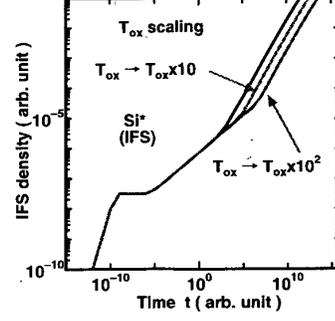


Figure 7: The effects of  $T_{ox}$  on IFS kinetics.

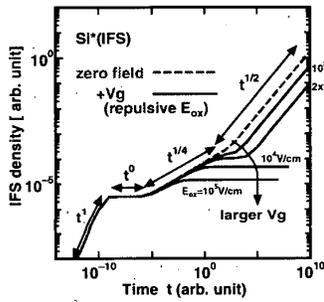


Figure 8: IFS kinetics with positively charged species; repulsive e-field.

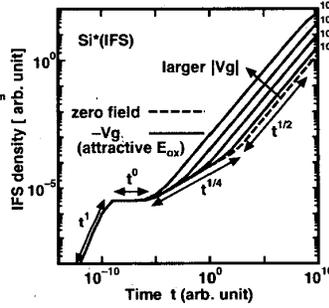


Figure 9: IFS kinetics with positively charged species; attractive e-field.

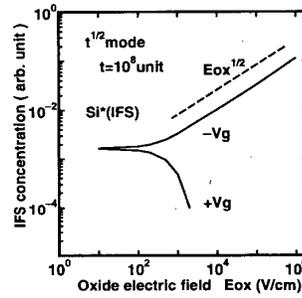


Figure 10: IFS kinetics with positively charged species; IFS concentration at  $t=10^8$  unit.

$L_{Rd}C_{IFS} = -J_{H,I} dt \quad (\text{transport limited})$ $= -A_I C_{H,I} dt \quad (\text{analytical solution for } J_{H,I} \text{ from Eqn. 3 in Fig. 1; uniform } J_H \text{ in the oxide; sink b.c. for } C_H.)$ $= A_I (k_G/k_R) C_{SH,0} / C_{IFS} dt.$ <p>(L.H.S. of Eqn. 1 in Fig. 1 set to 0 and <math>C_{SH} \simeq C_{SH,0}</math>)</p> $C_{IFS}(t) = 2^{1/2} L_R^{-1/2} A_I^{1/2} C_{SH,0}^{1/2} (k_G/k_R)^{1/2} t^{1/2},$	<p>where <math>A_I = D_H/T_{ox} \text{ Ber}(\mu_H E_{ox}/(D_H/T_{ox}))</math>.</p> $\text{Ber}(u) = u/(\exp(u) - 1),$ <p>when <math>u \rightarrow -\infty</math>, <math>\text{Ber}(u) \simeq  u </math>, when <math>u \rightarrow 0</math>, <math>\text{Ber}(u) \simeq 1</math>.</p> <div style="border: 1px solid black; padding: 5px; margin-top: 10px;"> <math display="block">C_{IFS}(t) \propto t^{1/2} \quad (0.5 \text{ power law of } t)</math> <math display="block">C_{IFS}(t) \propto  E_{ox} ^{1/2} \quad (\text{strong negative e-field limit})</math> <math display="block">C_{IFS}(t) \propto (D_H/T_{ox})^{1/2} \quad (\text{neutral species})</math> </div>
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Figure 11:  $t^{1/2}$  mode; analytical solution.