

## New Multi-stages – Hydrogen Diffusion Model for Negative Bias Temperature Instability

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In the present paper, we propose a new and physically based model for the negative bias temperature instability. The proposed model can predict the most accepted features of the degradation such as fast degradation recovery, as well as the long term recovery component. The field of negative bias temperature instability is filled with models proposed by many research groups. Most reliable models converge around the fact that the degradation is originated from two components; one of them is rapidly created and annealed whereas the other is permanent. However, these reliable models diverge on the microscopic nature of the two components and on the relation between them, especially whether they are correlated or not. Hydrogen,  $E'$  center, and Pb center are the most cited oxide defects to be the microscopic origin of the degradation. The fact that reliable and accurate studies end in contradicting results leads us to think that the origin of negative bias temperature instability degradation is the same thing seen from different angles. In this spirit, our model reconciles the two widely and experimentally proved features, which are hydrogen diffusion in the oxide, on one hand, and hole trapping and detrapping by oxide defects, on the other hand. This model predicts that both hydrogen and hole trapping/detrapping in the oxide defects play a key role in negative bias temperature degradation. The fast component is ascribed to hole trapping and detrapping in the oxide  $E'$  centers and interface dangling bonds generation. The permanent component is attributed to the  $E' - H$  complex and limited by the back diffusion of the hydrogen in the oxide to passivate Pb centers. One of the particularities of the proposed model is that the two components are both dependent (correlated) and independent (uncorrelated). During the stress period, the components are tightly coupled whereas during the long-term recovery the components are decoupled.

**Keywords:** NBTI, Bias instabilities, Holes trapping, Reaction-diffusion model, Two-stage model.

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### 1. INTRODUCTION

Negative bias temperature instability (NBTI) is one of the most longstanding reliability issues in CMOS technologies. Actually, NBTI is one of the major limiting factors of CMOS integration [1].

NBTI is the consequence of gradual and time-dependent buildup of positive charges in the substrate/oxide interface and/or in the gate insulator of a MOS based transistor under the application of negative bias and relatively high temperature. The generated positive charges cause a shift in transistor parameters such as threshold voltage, transconductance, sub-threshold slope, etc. [2]. Some of NBTI distinguishing signatures are the power law behavior during stress period and fast recovery alongside with long-term degradation that lasts for many decades [3].

Despite many attempts to model the degradation have been developed, none of them gets the consensus on the possible structures of the precursor defects. The proposed models can be classified as follows [4-7]:

1 One component is related to hydrogen instabilities in the oxide, which is often modeled by Reaction-Diffusion (RD) model;

2 One component is related to hole trapping/detrapping in the preexisting or stress-induced precursors;

3 Two independent components where the fast one is related to hole trapping/detrapping processes and the permanent one is due to hydrogen-related defects such as Pb-H and/or  $E' - H$  complexes;

4 Two independent components that result from generation and recovery of interface traps are modeled

by the RD model, together with hole trapping and detrapping in oxide defects;

5 Two independent components where the fast one is attributed to interface state passivation and the permanent one is ascribed to hole trapping in Deep-Level defects;

6 Two tightly coupled components where hole trapping in the oxide trigger  $E' - H$  complex formation by consuming Pb-H and leaving a dangling Pb center behind.

With the advance in measuring techniques of NBTI [8], the assumption of one component is abundant and most relevant results ascribe NBTI to two components; one permanent and the other recoverable. The relationship between the two components and their microscopic origin is under heavy debate. In general, NBTI models proposed in the literature are trying to answer the following questions:

– Q1: What are the microscopic origins of the two components? And which of them is permanent (slow) or recoverable (fast)?

– Q2: What is the relation (correlation) between the two components: coupled (dependent) or decoupled (independent)?

In this paper, we propose a new physical based model, which extends the two-stage model [7] to account the hydrogen diffusion in the oxide. The proposed model answers to the above mentioned two questions.

– The degradation is originated from Pb centers at the interface,  $E'$  centers in the oxide and  $E' - H$  complexes in the border of the Si-SiO<sub>2</sub> interface. The fast component is related to  $E'$  center trapping/detrapping,

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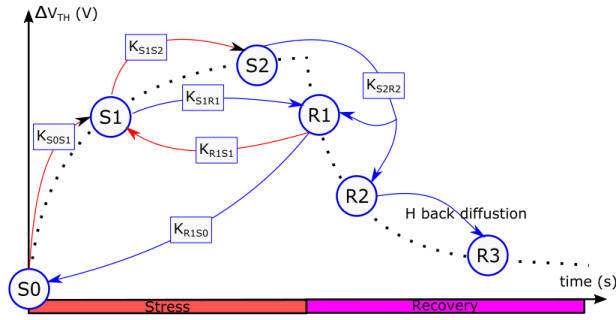
whereas the slow component is shared between  $E' - H$  complex and Pb centers.

– The two components are coupled and decoupled at the same time. They are tightly coupled during stress and fairly decoupled during recovery.

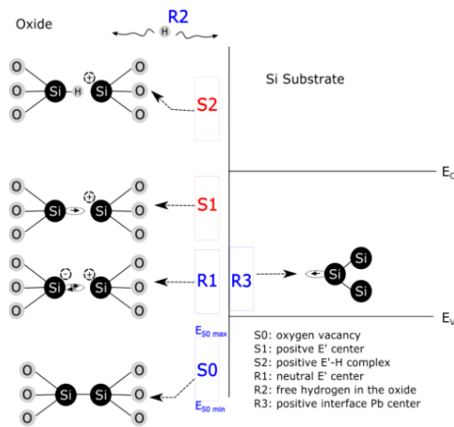
In the remaining of this article, we will discuss the steps to derive the mathematical equations of the model. In the model derivation way, we will highlight the microscopic components that are created and annihilated, and we will explain what we mean under coupled and decoupled at the same time. The validity of the model equations is checked using COMSOL Multiphysics simulator and results are discussed.

## 2. MODEL DERIVATION

Fig. 1 shows all dynamics of the proposed model and Fig. 2 illustrates the defects supposed to cause NBTI degradation highlighting their energy distribution with respect to the silicon substrate band gap. These two figures will be heavily referenced during our steps of model derivation.



**Fig. 1** – NBTI model dynamics: circles are stages of stress and rectangles are rate of transformation



**Fig. 2** – Defects involved in NBTI degradation and their energy distribution with respect to the silicon band gap

Dynamics and mathematical derivation of our model can be explained as follows.

### 2.1 Stress Period

During the stress period, the device is subjected to a negative bias under relatively high temperature. This period is characterized by the increase of channel hole concentration which plays a major role in oxide trap charging. In this developed model, the stress period

passes through three stages as depicted in Fig. 1.

**Stage zero of stress (S0):** this stage represents the device before stress. The NBTI related defect precursors are taken to be oxygen vacancies. Oxygen vacancies energy is distributed below the silicon upper valence band energy (S0 in Fig. 2). It is randomly distributed from 1.4 eV to 0.32 eV below the upper valence band [9].

**Stage one of stress (S1):** Upon application of the stress, substrate holes pile up near the Si-SiO<sub>2</sub> interface. Some of these holes acquire energy so that they have a non-negligible probability to tunnel to the nearby interfacial oxygen vacancies. Once an oxygen vacancy captures a hole, the bond between Si atoms is broken and hence one Si atom becomes a positive charge and the other stays neutral with one dangling bond. This new configuration of the oxygen vacancy is called  $E'$  center with a positive charge (S1 in Fig. 2).

The creation of  $E'$  center is accompanied by structural relaxation, which leads the energy level of the defect to shift. The energy of the newly created  $E'$  centers lays in the upper half of the Si band gap (S1 in Fig. 2). Within these energy levels,  $E'$  center has been positively charged and it will play a crucial role in the trapping/detrapping process of the proposed NBTI model.

By taking the oxygen vacancy concentration in the oxide to be  $N_{S0}$  [cm<sup>-3</sup>] and the newly created  $E'$  center to be  $N_{S1}$  [cm<sup>-3</sup>] (Subscript  $S$  represents stress; and 1, 2 for stage one and two respectively), the rate equations of transformation are given by:

$$\frac{dN_{S0}}{dt} = -K_{S0S1}N_{S0} \quad (1)$$

$$\frac{dN_{S1}}{dt} = K_{S0S1}N_{S0} \quad (2)$$

$$K_{S0S1} = p v_p^{th} \sigma_p e^{-\frac{x}{x_{p0}}} e^{-\beta \Delta E_{S0S1}} \theta(E_V - E_{S0}, e^{-\beta(E_V - E_{S0})}, 1) e^{\frac{F^2}{F_c^2}}$$

where  $K_{S0S1}$  is the rate of transformation from stage  $S0$  to stage  $S1$ ,  $p$  is the channel hole concentration,  $v_p^{th}$  is the hole thermal velocity,  $\sigma_p$  hole capture cross-section,  $\beta = 1/K_B T$ ,  $\Delta E_{S0S1}$  is the energy barrier that should be exceeded then a hole will be captured by oxygen vacancy,  $E_{S0}$  refers to the energy level of defects in state  $S0$ ,  $F$  is the electric field,  $F_c$  is the reference field for the multiphonon-field-assisted tunneling mechanism[7], and

$$\theta(E_{S0}, e^{-\beta E_{S0}}, 1) = \begin{cases} e^{-\beta E_{S0}} & E_V - E_{S0} \geq 0 \\ 1 & E_V - E_{S0} < 0 \end{cases}$$

It can be noted that these equations are preliminary and are subject to modification as long as the proposed model is derived.

**Stage two of stress (S2):** Being in state  $S1$ , hydrogen atoms bonded to the interfaces can move to the next  $E'$  center and form  $E' - H$  complex and leave behind it an interface dangling bond Pb center, which means that the formation of  $E' - H$  and Pb centers are tightly coupled [7]. The new created  $E' - H$  complex forms the permanent component of the NBTI.

Naming the  $E' - H$  concentration by  $N_{S2}$ , the rate of generation of the latter is:

$$\frac{dN_{S2}}{dt} = K_{S1S2}N_{S1}, \quad (3)$$

$$K_{S1S2} = \nu e^{(-\beta\Delta E_{S1S2} - E_{S2} - \gamma F)},$$

where  $K_{S1S2}$  is the rate of transformation from stage  $S1$  to stage  $S2$ ,  $\nu$  is the attempt frequency,  $\Delta E_{S1S2}$  is the energy barrier that a hydrogen bond should overpass to form the  $E' - H$  complex,  $E_{S2}$  is energy level of defects in the  $S2$  state and  $\gamma$  is the field acceleration parameter.

Now, the rate of change of  $N_{S1}$  in equation (2) becomes:

$$\frac{dN_{S1}}{dt} = K_{S0S1}N_{S0} - K_{S1S2}N_{S1} \quad (4)$$

At the end of the stress period, three types of positive charges are created:

- $E'$  centers: created during stage  $S1$ ;
- $E' - H$  centers: created during stage  $S2$ ;
- $N$  it interface states or Pb centers: created during stage  $S2$ .

The created  $E' - H$  centers and Pb centers are tightly coupled. Fig. 2 shows the energy distribution inside the oxide band gap.

## 2.2 Relaxation (Recovery) Period

During recovery, the stress is removed and eventually a positive voltage can be applied. The relaxation period is featured by the increase of substrate electron concentration in the channel which will play a major role in trap discharging.

**Stage one of relaxation (R1):** After removing the stress, electrons pile up at the substrate channel. Some of these electrons can rapidly tunnel back to the positive  $E'$  (stage  $S1$ ) center and neutralize it. The capture of an electron by  $E'$  center shifts the energy level of the trap down near to the upper band of the silicon valence.

Being in this stage, a neutral  $E'$  center can rapidly capture a hole from the valence band and becomes again positively charged and its energy level shifts up.  $E'$  center switches between two states: positively charged if it captures a hole or neutral if it captures an electron.

Taking  $N_{R1}$  to be the concentration of neutral  $E'$  center in stage  $R1$  ( $R$  stands for relaxation and 1 for stage one), the rate of change of  $N_{R1}$  is:

$$\frac{dN_{R1}}{dt} = K_{S1R1}N_{S1} - K_{R1S1}N_{R1} \quad (5)$$

where  $K_{S1R1}$  and  $K_{R1S1}$  are the rates of transformation from stage  $S1$  to stage  $R1$  and back from  $R1$  to  $S1$  respectively which can be written as follows:

$$K_{S1R1} = n\nu_p^{th} \sigma_n e^{-\frac{x}{x_{n0}}} e^{-\beta\Delta E_{S1R1}} \theta(E_{S1} - E_C, e^{-\beta(E_{S1} - E_C)})$$

and,

$$K_{R1S1} = p\nu_p^{th} \sigma_p e^{-\frac{x}{x_{p0}}} e^{-\beta\Delta E_{R1S1}} \theta(E_V - E_{R1}, e^{-\beta(E_V - E_{R1})})$$

For this stage, equation (4) becomes:

$$\frac{dN_{S1}}{dt} = K_{S0S1}N_{S0} - K_{S1S2}N_{S1} - K_{S1R1}N_{S1} + K_{R1S1}N_{R1}$$

In this stage, an  $E'$  center that does not capture a hole for a long time can recover back to an oxygen vacancy.

Taking this into consideration equations (1) and (5) we obtain:

$$\frac{dN_{S0}}{dt} = -K_{S0S1}N_{S0} + K_{R1S0}N_{R1}$$

and,

$$\frac{dN_{R1}}{dt} = K_{S1R1}N_{S1} - K_{R1S1}N_{R1} - K_{R1S0}N_{R1}, \quad (6)$$

where  $K_{R1S0}$  is the rate of transformation from stage  $R1$  to stage  $S0$ , which is given by:

$$K_{R1S0} = \nu e^{-\beta\Delta E_{R1S0}}.$$

**Stage two of relaxation (R2):** Electrons in the channel, depending on the temperature and the positive bias voltage, can acquire the necessary energy to overcome the energy barrier and capture the positive  $E' - H$  centers.

Being in the neutral state,  $E' - H$  complex has a non-zero probability to be dissociated and release its hydrogen in the oxide.

We argue that a positive  $E' - H$  complex has a neglected probability to release hydrogen in the oxide. Effectively, when the  $E' - H$  complex captures an electron from the silicon channel, the probability of releasing its hydrogen increases. This fact can be understood based on quantum mechanics principles.

The captured electron is located near the positively charged Si atom of the Si-H complex. According to quantum mechanics, the captured electron has a non-zero probability to be near the Si atom that is passivated by the hydrogen. Where the electron weakens the Si-H bond and hydrogen can be released into the oxide due to thermal agitation. After releasing the hydrogen, the  $E' - H$  complex returns back to a neutral  $E'$  center (see stage  $R1$  in Fig. 1 and Fig. 2).

Naming the species at this stage by  $N_{R2}$  (hydrogen atoms in the oxide), the rate of change of  $N_{R2}$  is given by:

$$\frac{dN_{R2}}{dt} = K_{S2R2}N_{S2}, \quad (7)$$

$$K_{S2R2} = n\nu_p^{th} \sigma_n e^{-\frac{x}{x_{n0}}} e^{-\beta\Delta E_{S2R2}} \theta(E_{S2} - E_C, e^{-\beta(E_{S2} - E_C)}).$$

And equations (3) and (6) will be rewritten as:

$$\frac{dN_{S2}}{dt} = K_{S1S2}N_{S1} - K_{S2R2}N_{S2},$$

$$\frac{dN_{R1}}{dt} = K_{S1R1}N_{S1} - K_{R1S1}N_{R1} - K_{R1S0}N_{R1} + K_{S2R2}N_{S2}.$$

**Stage three of the relaxation (R3):** The released hydrogen can diffuse into the oxide or came back and passivate a silicon–oxide interfacial dangling bond. The behavior is similar to what the RD model is in the recovery phase [10].

Equation (7) becomes:

$$\frac{dN_{R2}}{dt} = K_{S2R2}N_{S2} + D_H \frac{d^2N_{R2}}{dx^2} - K_r N_{it} D_{R2} \text{ (at } x = 0),$$

where  $D_H$  is the hydrogen diffusion coefficient in the oxide,  $K_r$  is the back interface reaction as defined in the context of RD model,  $N_{it}$  is the interface state concentration.

At the end of this relaxation period, the recovery of NBTI is the sum of three independent processes:

- 1- The capture of substrate electrons by positive  $E'$  centers (stage R1);
- 2- The capture of high energy electrons by the positive  $E' - H$  centers (stage R2); and
- 3- The back diffusion of hydrogen in the oxide to passivate a Pb center (stage R3).

The final equations of the developed model are:

$$\frac{dN_{S0}}{dt} = -K_{S0S1}N_{S0} + K_{R1S0}N_{R1}$$

$$\frac{dN_{S1}}{dt} = K_{S0S1}N_{S0} - K_{S1S2}N_{S1} - K_{S1R1}N_{S1} + K_{R1S1}N_{R1}$$

$$\frac{dN_{S2}}{dt} = K_{S1S2}N_{S1} - K_{S2R2}N_{S2}$$

$$\frac{dN_{R1}}{dt} = K_{S1R1}N_{S1} - K_{R1S1}N_{R1} - K_{R1S0}N_{R1} + K_{S2R2}N_{S2}$$

$$\frac{dN_{R2}}{dt} = K_{S2R2}N_{S2} + D_H \frac{d^2N_{R2}}{dx^2} - K_r N_{it} D_{R2} \text{ (at } x = 0)$$

The quantity of  $N_{it}$  can be obtained from:

$$\frac{dN_{it}}{dt} = -K_{S1S2}N_{S1} + K_r N_{it} N_{R2}$$

The total shift of the threshold can be evaluated by:

$$\Delta V_{TH} = -\frac{q}{C_{ox}} \left( \int_0^{t_{ox}} \left( 1 - \frac{x}{t_{ox}} \right) (N_{S1} + N_{S2}) dx + N_{it} \right)$$

The final answers to the two questions initiated in the introduction section are:

A1: The fast component is originated from the switching behavior of  $E'$  center. Positive  $E'$  centers are created during stage S1 and annealed during stage R1. Whereas the slow component is originated from  $E' - H$  and Pb centers. The  $E' - H$  and Pb centers are created during stage S2 and annealed during stage R2 for  $E' - H$  and stage R3 for Pb centers.

A2: The creation of  $E' - H$  and Pb centers is highly correlated with the creation of  $E'$  centers ( $K_{S1S2}$  transformation) during stress period. Whereas annealing of  $E'$ ,  $E' - H$  and Pb centers is totally independent processes, they are annealed during relaxation stage R1, R2 and R3 respectively.

### 3. RESULTS AND DISCUSSION

To validate the developed model, numerical simulations on a pMOSFET structure with an oxide thickness of 4 nm have been performed using COMSOL Multi-

physics simulator [12]. Defect energy distribution and barriers between states are predefined to follow a random uniform distribution (except for the S1-S2 transition barrier for which it uses Gaussian-like Fermi-derivative distribution) [9]. Table 1 gives the values of energy distribution and barriers between stages as used in these simulations.

The predictability of our model is investigated against some of the most accepted features of NBTI in the literature.

#### 3.1 Fast Recovery and Long Term Recovery

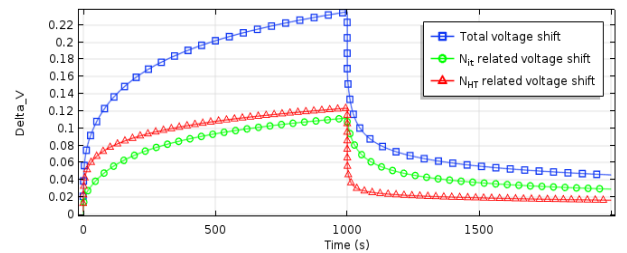
Fig. 3 shows the threshold voltage shift ( $\Delta V_{th}$ ) evolution during the stress at  $-1.5$  V and relaxation at 0 V. The total NBTI threshold voltage shift is the result of the superposition of interface trap generation contribution and oxide hole trapping contribution for stress period, and interface passivation and hole detrapping for the recovery period.

The generation of interface state is strongly coupled to the  $E' - H$  complex generation rate which results from the transfer from stage S1 to stage S2. This correlation between  $N_{it}$  and  $E' - H$  is lost during recovery period because the released hydrogen (the byproduct of S2 to R2 transformation) can diffuse freely into the oxide and only hydrogen atoms at the interface are responsible for interface passivation.

Our model predicts that the long-term NBTI recovery is limited by the diffusion of the hydrogen atoms towards the interface in concordance with many experimental results that highlight the role of hydrogen diffusion in NBTI degradation. In contrast to our model, the Two-Stage model fails to predict this long-term recovery of NBTI [7].

**Table 1** – Energy distribution and barrier used in simulation

Stage	Energy spread [eV]		Barrier	Energy spread [eV]	
	$E_{min}$	$E_{max}$		$E_{min}$	$E_{max}$
S0 (Oxygen vacancy)	$E_{S0}$ min	-1.14	S0S1	$E_{S0S1}$ min	0.01
	$E_{S0}$ max	-0.31		$E_{S0S1}$ max	1.14
S1 (positive $E'$ center)	$E_{S1}$ min	0.57	S1S2	$E_{S1S2}$ mean	1.46
	$E_{S1}$ max	1.11		$E_{S1S2}$ std. dev	0.44
S2 ( $E' - H$ complex)	$E_{S2}$ min	1.13	S1R1	$E_{S1R1}$ min	0.4
	$E_{S2}$ max	2.13		$E_{S1R1}$ max	0.4
R1 (neutral $E'$ center)	$E_{R1}$ min	0.1	R1S1	$E_{R1S1}$ min	0.4
	$E_{R1}$ max	0.55		$E_{R1S1}$ max	0.4
R2 (free hydrogen)	–	–	R1S0	$E_{R1S0}$ min	0.7
	–	–		$E_{R1S0}$ max	1.2
R3 (Pb centers)	–	–	S2R1	$E_{S2R1}$ min	0.3
	–	–		$E_{S2R1}$ max	0.9



**Fig. 3** – Time evolution of threshold shift for 1000 s of stress at  $-1.5$  V followed by 1000 s of recovery at 0 V

Alongside with the long-term recovery prediction capability of our model, it also succeeded in reproducing the fast early recovery of the degradation. It is the fast switch between Stage *S1* and Stage *R1* and back forth that is the behind the fast recovery of the NBTI.

### 3.2 Power Law and Time Exponent

Our model predicts that the NBTI degradation follows a power law characteristic with time exponent of 0.26 as illustrated in Fig. 4. Although a 0.25 time exponent is reported in the literature, the 0.16 time exponent is the most accepted by researchers in the field especially after the introduction of ultra-fast measurement technique and on-the-fly ones.

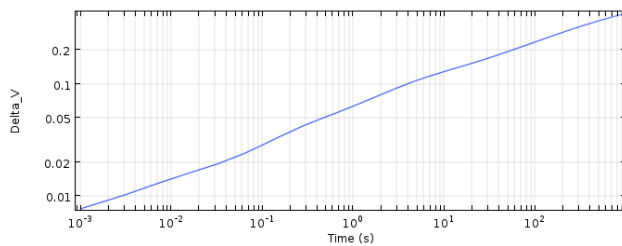


Fig. 4 – Threshold shift in a log-log scale. The extract power law time exponent is 0.26

### 3.3 Stress Voltage and Temperature Dependence

Fig. 5 and Fig. 6 show that our model is able to predict the stress voltage sensibility of the NBTI degradation as well as its temperature dependence. The stress voltage dependence is attributed to the  $\exp(F^2/Fc^2)$  in the rate of transformation from *S0* to *S1*, whereas the temperature dependence of the NBTI is included in the energy barriers that should be exceeded to transit between stages.

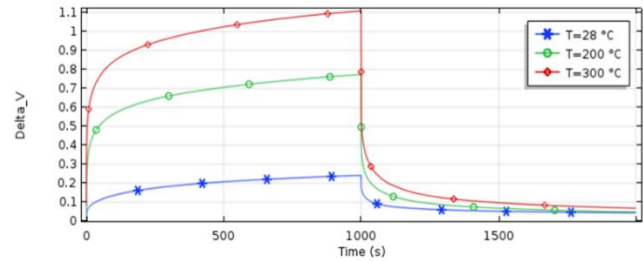


Fig. 5 – NBTI degradation for different voltage stress at  $T = 200 \text{ }^\circ\text{C}$

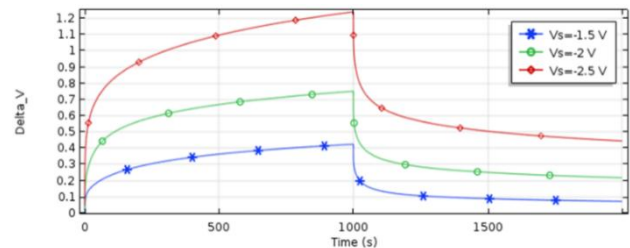


Fig. 6 – NBTI degradation for different temperatures at  $V_s = -1.5 \text{ V}$

## 4. CONCLUSIONS

The dynamics and mathematical derivation of our model have been presented. The model predicts that both hydrogen and hole trapping-detrapping play a major role in NBTI degradation. The generation of the  $E' - H$  complex is a consequence of the transformation from state *S1* to *S2*, which is tightly coupled to substrate hole trapping in  $E'$  center. The fast component of NBTI degradation is caused by the switching character of  $E'$  centers. Whereas the permanent part of the degradation is ascribed to the  $E' - H$  complex and hydrogen back diffusion in the oxide.

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## Нова багатоступенева модель дифузії водню для негативного зміщення температурної нестабільності

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У цій статті пропонується нова фізично обґрунтована модель для негативного зміщення температурної нестабільності (NBTI). Запропонована модель може передбачити найбільш прийнятні ознаки виродження, такі як швидке відновлення виродження, а також компоненти тривалого відновлення. Поле негативного зміщення температурної нестабільності описується моделями, запропонованими багатьма дослідницькими групами. Більшість надійних моделей сходяться навколо факту, що виродження відбувається з двох компонентів. Однак ці надійні моделі розходяться за мікроскопічним характером двох компонентів і за зв'язком між ними, особливо незалежно від того, корельовані вони чи ні. Водень,  $E'$  центр, і Pb центр є найчастіше згадуваними оксидними дефектами, які є мікроскопічним джерелом виродження. Той факт, що надійні і точні дослідження закінчуються суперечливими результатами, змушує нас думати, що причина негативного зміщення температурної нестабільності – це те ж саме, що видно під різними кутами. У цьому дусі наша модель поєднує дві широко і експериментально доведені особливості: дифузію водню в оксиді, з одного боку, і захоплення та видалення дірок оксидними дефектами, з іншого боку. Ця модель передбачає, що як захоплення, так і вивільнення водню і дірок в оксидних дефектах грають ключову роль в негативному зміщенні температурної нестабільності. Швидка складова пов'язана із захопленням і вивільненням дірок в оксидних  $E'$  центрах і появою обірваних зв'язків на межі розділу. Постійний компонент відноситься до комплексу  $E' - H$  і обмежений зворотною дифузією водню в оксиді для пасивації центрів Pb. Одна з особливостей запропонованої моделі полягає в тому, що обидва компоненти є залежними (корельованими) і незалежними (некорельованими). Протягом робочого періоду компоненти тісно пов'язані між собою, тоді як під час тривалого відновлення компоненти не пов'язані між собою.

**Ключові слова:** NBTI, Нестабільність зміщення, Захоплення дірок, Реакційно-дифузійна модель, Двоступенева модель.