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A Computational Model of NBTI and Hot Carrier Injection Time-Exponents for MOSFET Reliability

HALDUN KUFLUOGLU AND MUHAMMAD ASHRAFUL ALAM
School of Electrical and Computer, Engineering 1285 Electrical Engineering Building, Purdue University, West Lafayette, IN 47907-1285, USA
haldun@purdue.edu

Abstract. Theories of interface trap generation in Negative Bias Temperature Instability (NBTI) and Hot Carrier Injection (HCI) mechanisms are unified under the geometric interpretation and computational modeling of Reaction-Diffusion (R-D) theoryframework. Analytical derivations that predict the degradation are shown, simulation methodology is explained and numerical solutions are obtained. Time-exponents and degradation behavior under dynamic bias in agreement with experimental observations are discussed. Implications regarding ultra-scaled surround-gate device structures are presented.

Keywords: MOSFET, reliability, NBTI, HCI, reaction diffusion, surround-gate

1. Introduction

In conventional MOSFETs, the gate oxide, an amorphous material, is grown over the perfectly-crystalline Si channel. Thus, at the semiconductor-oxide interface, some of the Si bonds remain dangling and can act as precede interface traps. These traps yield poor device characteristics, therefore during manufacture, the transistors are annealed in hydrogen ambient so that the gas diffuses into the oxide and passivates the interface traps, forming Si─H bonds. This traditional method proved to be an effective solution to the interface trap instabilities for decades; however the continuing MOSFET miniaturization trends, (i.e., aggressive oxide thickness scaling and process modifications such as employing nitrided oxides to prevent boron penetration from the poly-gate) accelerate bond-breaking at the interface over time during the device operation. The traps shift the threshold voltage, reduce the channel mobility due to scattering and induce parasitic capacitances in the transistors. Overall, the drain current degrades and parametric reliability becomes a significant concern.

The most important mechanisms that break the Si─H bonds at the Si/oxide interface are Negative Bias Temperature Instability (NBTI) and Hot Carrier Injection (HCI). NBTI is dominant in PMOSFETs whereas HCI is the major degradation mechanism in NMOSFETs.

NBTI occurs in negatively biased transistors at elevated temperatures. The inversion layer holes can tunnel into the oxide and their interaction with passivated Si atoms can break the Si─H bond leaving behind the interface trap, and the associated H atom diffuses away from the Si/oxide interface. The cold holes in the channel can tunnel into the gate oxide independent of their channel location; therefore the trap distribution is uniform over the channel in NBTI.

In hot carrier injection process, the electrons accelerated in the lateral electric field of the channel impact ionize and generate hot electron-hole pairs. The injection of these carriers into the oxide breaks the Si─H bonds. Since the impact ionization is concentrated towards the drain side, HCI damage is localized compared to NBTI degradation.

Traditionally, NBTI and HCI have been treated separately due to the differences in time-behaviors (Fig. 1) and the physics of bond-breaking at the interface. However, both phenomena include broken Si─H bonds and diffusion of H through the oxide, therefore a common theoretical framework should be able to explain both phenomena. Since the trap distribution in NBTI is

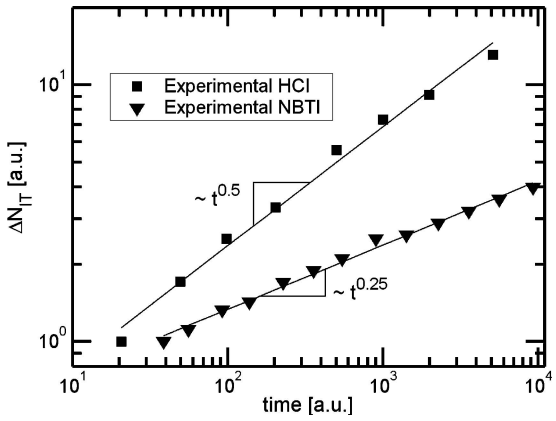

Figure 1. Experimental interface trap density (N_{IT}) shows characteristic time-dependecies for NBTI and HCI. NBTI increase as $t^{0.25}$ whereas HCI damage evolves as $t^{0.5}$. V_T, I_{dsat} and I_{dlin} behave similar to N_{IT}. Data from [1,2].

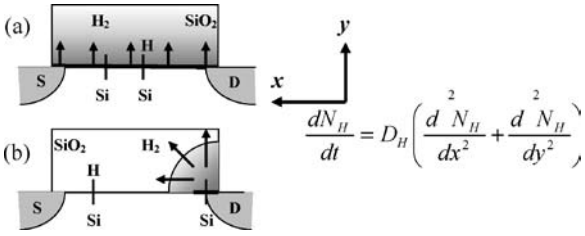

Figure 2. Hydrogen diffusion in oxide for NBTI and HCI mechanisms. HCI is localized near the drain, therefore the diffusion is 2-D. The diffusion equations reflect the geometric difference.

uniform, H diffusion is of 1-D nature, but HCI damage is localized near the drain end, so the diffusion is 2-D as shown in Fig. 2(b). We show that this geometry dependence of degradation is a key to understanding the different rate of degradation of NBTI and HCI.

In this paper, we explore geometry of the hydrogen diffusion using a computational analysis and explain the time-dependencies of NBTI and HCI under a unifying theoretical model. We derive the analytical equations, then obtain numerical solutions and compare with experimental observations. Finally, we consider the implications of our model for future-generation surround-gate transistor geometries.

2. Reaction-Diffusion Model

NBTI time-evolution has been successfully explained by the Reaction-Diffusion (R-D) framework [3,4]. In this model, the bond-breaking at the interface is represented as the chemical reaction given in (1)

$$\text{Si} - \text{H} + h^+ \rightleftharpoons \text{Si}\bullet + \text{H}^o. \tag{1}$$

The net rate of increase in interface trap density is

$$\frac{dN_{IT}}{dt} = k_f(N_0 - N_{IT}) - k_r N_{IT} N_H^{(0)}, \tag{2}$$

where k_f and k_r are the forward and reverse reaction rates of (1), respectively. N_0 is the maximum density of Si—H bonds available and $N_H^{(0)}$ is the hydrogen density at the Si/oxide interface. The generation rate is a competition between the bond-breaking and the annealing terms.

After sufficient hydrogen build-up at the interface, H begins to diffuse into the oxide. The diffusion process removes H from the interface, therefore the reaction in (1) proceed in the forward direction during the stress, and thus the diffusion rate limits the interface trap generation rate.

Since every trap correspond to one H in the oxide, and $N_H(r)$ in NBTI can be approximated as in Fig. 3(a),

$$N_{IT}(t) = \int_0^{\sqrt{D_H t}} N_H(y,t)dy, \tag{3}$$

$$= N_H^{(0)}\sqrt{D_H t}, \tag{4}$$

and substituting (3) into (2) and assuming relatively slow generation of interface traps under steady-state conditions ($dN_{IT}/dt \sim 0$), we find

$$N_{IT}(t) = \sqrt{\frac{k_f N_0}{k_r}} \cdot (D_H t)^{0.25}. \tag{5}$$

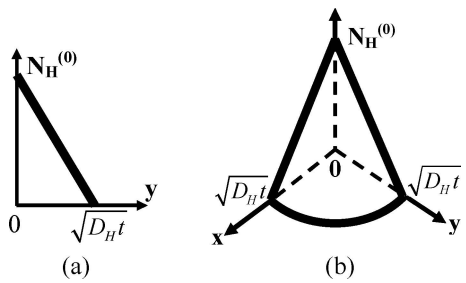

Figure 3. The hydrogen diffusion in the oxide. (a) In NBTI, 1-D hydrogen diffusion is approximated as a triangular profile. (b) The diffusion is 2-D in HCI, therefore N_H has a conical form.

From (4), the time-exponent of NBTI is independent of the bond-breaking mechanism and only depends on the diffusion of hydrogen. Modifying (3) for 2-D hydrogen diffusion in HCI and using $N_H(r)$ as shown in Fig. 3(b),

$$N_{IT}(t) = \frac{\pi}{2}\int_0^{\sqrt{D_H t}} N_H(r,t) r dr \tag{6}$$

$$\approx \sqrt{\frac{k_f N_0}{k_r}} \cdot (D_H t)^{0.5} \tag{7}$$

predicts the experimentally observed time-exponent $n = \frac{1}{2}$ [5].

3. Numerical Implementation

The geometry-aware R-D model is solved through a time-dependent Newton's Method implementation. The discretization scheme of the simulation domain is shown in Fig. 4.

The diffusion of hydrogen in 2-D is implemented in cylindrical coordinates. A schematic of the Jacobian matrix, is shown in Fig. 5. The hydrogen and interface trap densities are computed simultaneously. The term a_R couples the interface density to the hydrogen density at the Si/oxide interface through the rate Eq. (2). Correspondingly, the a_{BC} term represents the boundary condition derived from box-integration given in (8–10).

In the oxide,

$$\frac{\partial N_H}{\partial t} = \nabla \cdot F_H, \tag{8}$$

where $F_H (= D_H \nabla N_H)$ is the hydrogen flux. Integrating (8) at the Si/oxide interface as in (9) gives the boundary condition in (10)

$$\frac{\partial}{\partial t}\int_{r_0}^{r_0+h/2} N_H r dr = \int_{r_0}^{r_0+h/2} (\nabla \cdot F_H) r dr \tag{9}$$

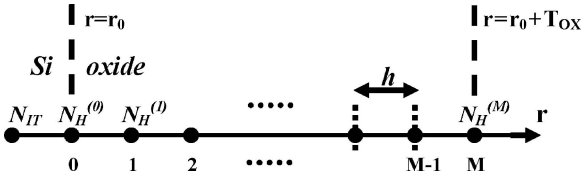

Figure 4. The gate oxide is discretized uniformly. The N_{IT} term is at the Si/oxide interface, directly communicating with the $N_H^{(0)}$ node.

$$\mathrm{J} = \begin{bmatrix} \begin{pmatrix} a_{N_H^M} & \cdots & \cdot \\ \vdots & \ddots & \vdots \\ \cdot & \cdots & a_{N_H^0} \end{pmatrix} & a_{BC} \\ a_R & \{a_{N_{IT}}\} \end{bmatrix}$$

Figure 5. The Jacobian matrix, J, contains the hydrogen diffusion block and the interface trap density term. Both are coupled through the chemical reaction terms and the boundary condition at the Si/oxide interface. The matrix is tri-diagonal when implemented in cylindrical coordinates.

$$\frac{h}{2}\cdot\frac{\partial N_H}{\partial t} = \left(\frac{2r_0+h}{2r_0+\frac{h}{2}}\right)\left[D_H\frac{\partial N_H}{\partial r} - \left(\frac{2r_0}{2r_0+h}\right)\frac{dN_{IT}}{dt}\right] = 0. \tag{10}$$

Grid-spacing h and inner radius r_0 are defined in Fig. 4. At the gate/oxide interface, the boundary condition assumes infinite diffusion velocity. Exponentially-increasing time steps are utilized to simulate time periods comparable to the lifetimes of the transistors (e.g., approximately, i.e., about 10 years). The simulation can also be implemented in Cartesian coordinates. The matrix J has additional off-diagonal elements, and the boundary conditions need to be derived properly for convergence.

4. Simulation Results

Figure 6 shows the numerical solutions of the R-D model for NBTI and HCI. In the diffusion dominated regime, 2-D HCI simulation clearly demonstrates the anticipated time-slope. In Fig. 7, the simulation results compared with experimental HCI time-exponents capture the general trend of the data.

5. Implications

Geometrically modified R-D model that explains the HCI degradation in planar structures can also be used to interpreted for NBTI of non-planar device structures. Surround-gate transistors like geometry that is representative of nanowire MOSFETs, VRG transistors or FINFETs. and Predicted NBTI time-dependence

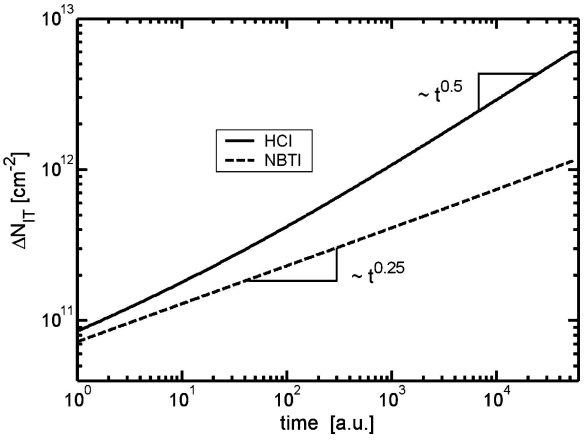

Figure 6. Numerical solutions of the R-D model for NBTI and HCI. HCI clearly shows the expected $t^{0.5}$ behavior during H diffusion.

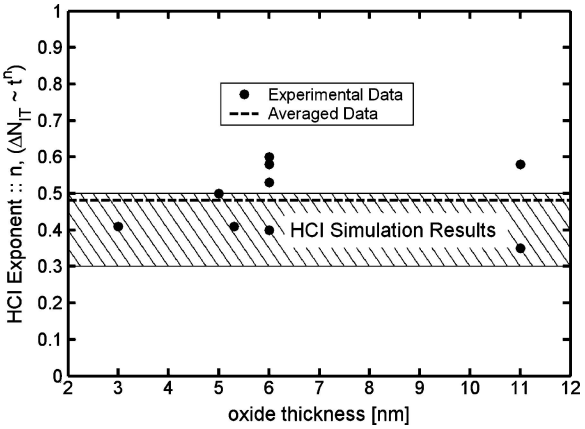

Figure 7. Comparison of HCI simulation results with the time-exponents compiled from [6–9]. The hatched region follows the general trend of the data.

of such structures are presented in Fig. 8(a) and (b), respectively. As the transistor is scaled, the hydrogen diffusion behavior is shifted from 1-D to 2-D, and the degradation increases significantly. Facet dependent N_0 in (5) can also increase degradation, but the time-exponent does not change [10]. Therefore, the model implies worsened NBTI degradation (for a given V_G) for such transistor structures purely due to the device geometry. for such transistor structures purely due to the device geometry. However, if better electro-static control of surround-gate devices allow operation at lower V_G, the devices could still have an overall reliability advantage compared to planar devices.

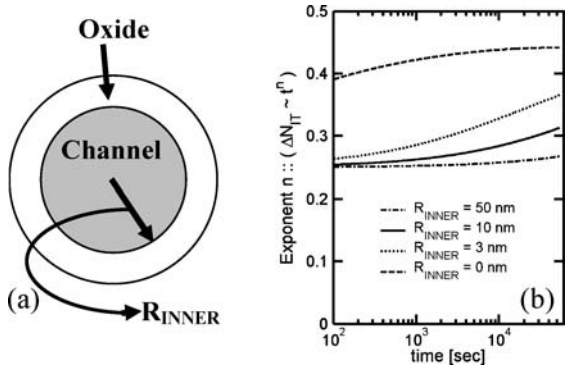

Figure 8. (a) Schematic of a cylindrical MOSFET cross section. The channel is surrounded by the gate oxide. A planar MOSFET can be imagined as $R_{\mathrm{INNER}} \rightarrow \infty$. (b) Assuming same V_D and T_{OX}, NBTI degradation of the surround-gate device increases significantly as the transistor is scaled. The time-exponent approaches $n = 0.5$, signaling the HCI-like hydrogen diffusion.

6. Conclusion

Time-dependent behavior of NBTI and HCI induced interface trap generation are unified by developing a geometry-aware Reaction-Diffusion model. It was found that the time-exponents of the degradation mechanisms stem from the diffusion of hydrogen in the oxide, and not from the distribution of Si—H bond-strengths at the Si/oxide interface. Numerical solutions consistent with the experimental observations are obtained. For surround-gate device geometries, the model predicts worsened NBTI degradation as the transistors are scaled down.

Acknowledgment

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