B-4-2
Mechanism of Threshold Voltage Shift (ΔV\text{th}) Caused by Negative Bias Temperature Instability (NBTI) in Deep Sub-Micron pMOSFETs

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1. Introduction
Negative bias temperature instability (NBTI) has become more serious as the dimension of CMOS devices is continually scaled. It's been reported that when the oxide thickness is less than 3.5 nm, the threshold voltage shift (ΔV\text{th}) of pMOSFET due to NBTI becomes to limit the device lifetime [1]. Although much effort has been recently dedicated to the study of NBTI [1-5], the details of the degradation process are not well understood. However, a good understanding of the physical mechanism responsible for NBTI is basic to the minimization of this degradation mode, which is the objective of this work.

2. Physical Model of NBTI Mechanism
The physical model to be presented is based on the structure of the SiO\text{2}/Si interface, as schematically depicted in Fig. 1, and the electrochemical reactions at the SiO\text{2}/Si interface given by the following [2]:

\[ \text{Si} + 2\text{H}^+ + 2e^- \rightarrow \text{SiH}_2^+ \] (1)

\[ \text{Si} + \text{H}^+ + e^- \rightarrow \text{SiH} \] (2)

\[ \text{H}_2\text{O} \rightarrow \text{H}^+ + \text{OH}^- \] (3)

where \text{Si} is a hydrogenated trivalent silicon, A is a neutral water-related species at the SiO\text{2}/Si interface, \text{p} is a hole at the silicon surface, \text{SiH} is a neutral trivalent silicon (i.e. interface state), and \text{H}^+ is a positively charged interstitial hydrogen ion. Briefly speaking, during NBTI, positive hydrogen ions are released from the hydrogen terminated silicon bonds by breaking the Si-H bonds. Some of the hydrogen ions diffuse away from the interface into the oxide bulk where some are trapped, causing threshold voltage shift. Hence, the threshold voltage shift can be expressed as:

\[ \Delta V_{\text{th}} = \Delta V_{\text{th,0}} + \Delta V_{\text{th,bulk}} \] (4)

where \Delta V_{\text{th,0}} is the initial threshold voltage shift at the interface and \Delta V_{\text{th,bulk}} is the threshold voltage shift due to the diffusion of hydrogen ions into the oxide bulk. Similar to the kinetics of trap filling and detrapping in the oxide [6-8], a first order time-dependent rate equation is used to model \Delta V_{\text{th}} due to NBTI. That is, for reaction (i),

\[ \frac{d\Delta V_{\text{th}}}{dt} = \frac{k[H^+ + \text{p}]}{t_f} - \frac{k[H^+ + \text{p}]}{t_r} \] (5)

where \( t_f \) and \( t_r \) are the time constant for forward reaction and reverse reaction, respectively.

Solving Eq. (4) and (5), \Delta V_{\text{th}}(t) can be obtained and is of the following form:

\[ \Delta V_{\text{th}}(t) = B_1[1 - \exp(-t/t_1)] + B_2[1 - \exp(-t/t_2)] \] (6)

where B_1 and B_2 are constant, and 1/t_1 = (1/t_f + 1/t_r) for reaction (i).

In the next section, it will be demonstrated that Eq. (6) can well describe the experimental data for NBTI.

3. Experimental Results and Discussions
The samples used in this study are P+ gate pMOSFETs with 3.3-nm or 2.2-nm gate oxide fabricated using a standard 0.18-μm or 0.13-μm CMOS process, respectively. The experimental arrangement for NBTI stress is illustrated in Fig. 2, in which the stress was interrupted at pre-determined stages to measure \( V_{\text{th}} \). Fig. 3(a) shows the threshold voltage shift (ΔV\text{th}) versus stress time (\( t \)) for three different stress gate biases at an elevated temperature of 175°C, and Fig. 3(b) for four different stress temperatures at a stress bias of -2.75V. Also included in Fig. 3 are the fitted curves using Eq. (6). The excellent agreement between the fitted curves and experiments shows the validity of the proposed model. The model is further verified, as shown in Fig. 4, by fitting the data taken from Ref. [5] for hydrogen and deuterium post-metal anneals. It's apparent that, from Figs. 3 and 4, \( \Delta V_{\text{th}} \) initially increases with stress time, and then tends to saturate after some stress time.

The time evolution of the threshold voltage shift is explained below. At the early stress stage, reaction (1) and (2) favor the generation of the interface states and the positive hydrogen ions at the interface, and the process is limited by the dissociation rate of the hydrogen terminated silicon bonds (i.e. reaction limited). However, after some stress time, the transport of hydrogen ions from the interface into the oxide bulk, i.e. reaction (3), limits the process and the diffusion rate is controlled by two factors: (a) gradually decreased field at the oxide/Si-substrate interface due to positive charges trapped in the oxide and (b) gradual increase in interface states that are favorable to the reverse reaction of (1) and (2). As a result, further diffusion of hydrogen ions is discouraged and therefore \( \Delta V_{\text{th}} \) becomes smaller and smaller with stress time (i.e. diffusion limited). Finally, \( \Delta V_{\text{th}} \) saturates when a dynamic balance is reached for each of reaction (1), (2), and (3).

4. Minimization of NBTI
According to the proposed model, the threshold voltage shift during NBTI stress originates from the electrochemical reaction (1) and (2) at the SiO\text{2}/Si interface, implying that the hydrogen terminated silicon bonds (\text{SiH}) at the SiO\text{2}/Si interface needs to be reduced in order to minimize the NBTI-induced device degradation. One way to achieve this is to introduce an appropriate amount of fluorine (F) by ion implantation into the gate oxide [9]. From Fig. 5, it's clear that the incorporation of F in the oxide effectively reduces NBTI. Another possible approach is to somehow increase the hardness of hydrogen terminated silicon bonds. For example, compared to the traditional hydrogen post-metal anneal (PMA), the use of deuterium PMA to passivate the dangling bonds can suppress the NBTI as shown in Fig. 4, because the bonds to deuterium are more difficult to break than bonds to hydrogen (known as kinetic isotope effect [10]).
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References


Fig. 1 Structure of the SiO₂/Si interface.

Fig. 2 Experimental arrangement for NBTI stress.

Fig. 3 Threshold voltage shift versus stress time under NBTI stress. The solid lines are fitted curves using Eq. (6).

Fig. 4 ΔVₚ vs. t under NBTI stress for hydrogen (H₂) and deuterium (D₂) post-metal anneals (PMA). The data points are taken from Ref. [5], and the solid lines are fitted curves using Eq. (6).

Fig. 5 ΔVₚ vs. t under NBTI stress for samples with or without F added to the oxide. The solid lines are fitted curves using Eq. (6).