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The role of hydrogen in negative bias temperature instability of pMOSFET*

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The NBTI degradation phenomenon and the role of hydrogen during NBT stress are presented in this paper. It is found that PBT stress can recover a fraction of $V_{\rm th}$ shift induced by NBTI. However, this recovery is unstable. The original degradation reappears soon after reapplication of the NBT stress condition. Hydrogen-related species play a key role during a device's NBT degradation. Experimental results show that the diffusion species are neutral, they repassivate Si dangling bond which is independent of the gate voltage polarity. In addition to the diffusion towards gate oxide, hydrogen diffusion to Si-substrate must be taken into account for it also has important influence on device degradation during NBT stress.

Keywords: negative bias temperature instability, device degradation, hydrogen diffusion, interface traps

PACC: 7340Q, 7300, 7220J

1. Introduction

As the MOSFET size is continuously scaled down without reducing supply voltages appropriately, its reliability has become more and more important in connection with hot carrier injection (HCI), time-dependent dielectric breakdown (TDDB) and negative bias temperature instability (NBTI).[1−3] NBTI in PMOS devices is the major reliability concern in modern CMOS technologies. An ultrathin gate oxide is essential for achieving high current drive in low power operation. The integrity and reliability of such thin-gate oxides are therefore crucial for ULSI manufacturing. Though first observed more than 30 years ago in nonvolatile memory devices, NBTI has now become an important reliability concern for mainstream digital, as well as analog CMOS circuits.[4] It results in threshold voltage ($V_{\rm th}$) shift, drain current degradation and transconductance decrease and becomes more severe as gate oxide is thinned down.

In general, NBTI is attributed to the generation of interface traps and fixed charges during stress in Si-substrate/oxide interface. Though a number of attempts have been made to investigate the mechanism of NBTI, no attempt has been made to explain the full experimental data within a common framework. The presence of hydrogen has long been thought to be critical for NBTI. It is believed to be the main passivating species for Si dangling bonds and plays a major role during NBT stress, when SiH bonds are depassivated and forming interface traps. Moreover, nitrogen incorporation into the gate dielectric may further exacerbate the issue. Hydrogen and its interaction with nitrogen in nitrided gate oxide are also a concern. Hydrogen is the most common impurity in MOS integrated circuits, being incorporated into the oxide during various phases of device fabrication, e.g., nitride deposition and forming gas anneal. Hydrogen can exist in its atomic state H^0, as molecular H_2, as positively charged hydrogen or proton H^+, as part of the hydroxyl group OH, as hydronium H_3O^+, or as hydroxide ions OH^-. More recent literature suggests that H^0 is unstable in both silicon and SiO_2 and is not expected to exist.[1] This paper presents an un-

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derstanding of the role of the hydrogen during NBT stress based on the degradation phenomenon of NBTI in pMOSFETs.

2. Experiments

Experiments were performed on surface channel LDD pMOSFETs and nMOSFETs, having t_{ox} of 3.2nm, width of 20μm and channel length of 0.18μm respectively. The gate oxides of all devices were annealed in N_2O atmosphere after thermal growth. All tests were complete by HP4156B high precision semiconductor parameter analyser in dry air. Stressing was performed at logarithmic time (t) intervals, which were periodically stopped to measure device characteristics. For all stress cases, the threshold voltage (V_{th}) was measured from I_d-V_g curve using maximum slope method with drain voltage –0.05V. The typical stress condition is illustrated in Fig.1. The device was stressed with constant negative gate voltage and temperature with the source, drain and substrate grounded. PBT stress was also performed if necessary, which stressed the device with a positive gate voltage whose absolute value is equal to that of NBTI. A fraction of NBTI degradation can be recovered by this PBT process, which benefits the improvement of the device lifetime under AC operation and also contributes to understanding the mechanism of NBTI. Typical stress temperature lies in 100°C–250°C range with oxide electric field typically below 6MV/cm, such field and temperature are typically encountered during burn in, but also approached in high performance IC's during routine operation.[1]

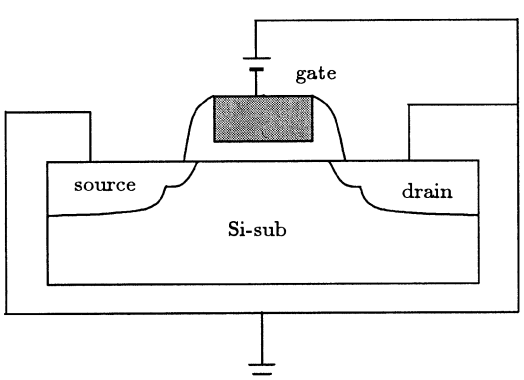


Fig.1. Configuration of stress condition.

3. Results and discussion

3.1. Device degradation during NBT stress

Either negative gate voltage or elevated temperature can degrade the device, but a stronger and faster effect is produced by their combined action. Fig.2 and Fig.3 show the devices' threshold voltage and saturated drain current degradation with time under various stress conditions respectively. The test devices are pMOSFETs and nMOSFETs with W/L=20μm/0.18μm under the stress voltage –2.75V and 2.75V at 100°C in dry air. It can be seen from these two figures that NBTI degradation in pMOSFETs is more serious than NBTI in nMOSFETs and PBTI in both nMOSFETs and pMOSFETs, which is consistent with previous researches.[4] Of all device parameters, V_{th} has the largest shift, in general V_{th} shift is considered as the criterion of NBTI degradation magnitude.

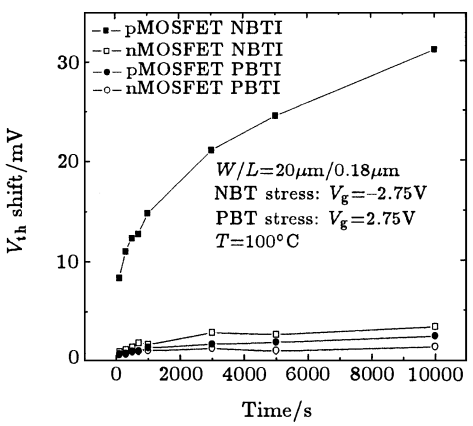


Fig.2. V_{th} shift of nMOSFET and pMOSFET as functions of stress time under NBT and PBT stress conditions with V_g=–2.75V and 2.75V respectively at 100°C for 10000s.

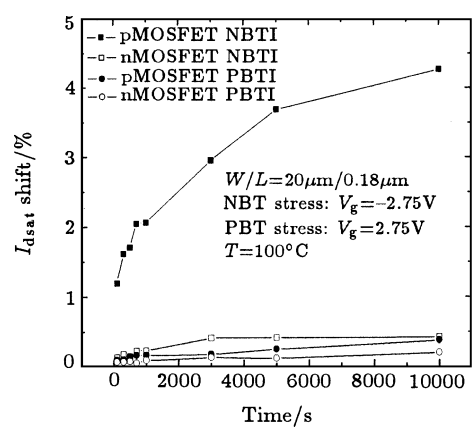


Fig.3. I_{dsat} shift of nMOSFET and pMOSFET as functions of stress time under NBT and PBT stress conditions with V_g=–2.75V and 2.75V respectively at 100°C for 10000s.

For a constant gate voltage stress, the threshold voltage shift ΔV_{th} is observed to depend on the stress

time t as t^a. Although different values of exponent a have been reported in literature, the commonly observed exponent is around 0.25. According to the widely accepted model, this suggests that the process could be controlled by the diffusion of hydrogen-related species from the Si-substrate/oxide interface, leaving behind charged interfacial states. These states are in turn responsible for device degradation and their density is directly proportional to the threshold voltage shift. These processes could be described by the following equations:

$$\mathrm{Si_3 - Si - H} \rightarrow \mathrm{Si_3 - Si^0 + X_{interface}}, \quad (1)$$

$$X_{\mathrm{interface}} \rightarrow X^{+}_{\mathrm{bulk}}. \quad (2)$$

Where $\mathrm{Si_3}$-$\mathrm{Si^0}$ represents interface traps and X represents species of hydrogen. First reaction (1) generates interface traps at the interface and then in reaction (2) the released hydrogen-related species diffuse into the gate dielectric and positive charges are generated. Both the donor interface traps and the fixed oxide charges contribute to the threshold voltage shift in the negative direction. This NBTI model is widely accepted. We also obtained the similar result with a typical curve given in Fig.4 with exponent 0.28.

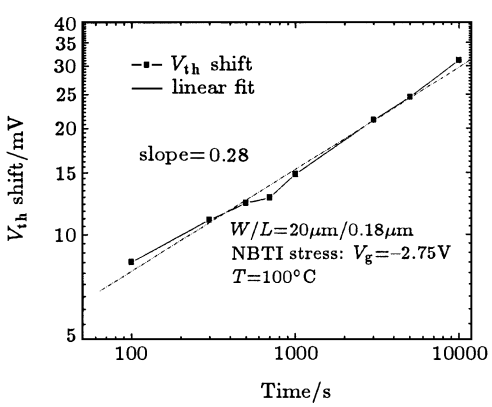


Fig.4. V_{th} shift of pMOSFET under V_{g}=–2.75V at 100°C for 10000s in log-log scale.

Figure 5 shows a saturated I_{d}-V_{g} curve in a semilog scale. Not only the drain current decrease but also the subthreshold slope increase after NBT stress can be seen in this figure, which means that interface traps are created during NBT stress at the Si-substrate/oxide interface. The gate current change is illustrated in Fig.6, we can see that there is a large increase after NBT stress, this is caused by the presence of interface traps and (or) oxide traps. These defects cause gate current increasing. Defect generation is one important reliability issue for MOSFETs. The generated defects have a number of adverse effects on the device, including shift in device parameters, stress induced leakage current (SILC), noise, and eventually the gate oxide breakdown. Defects can be formed in the bulk of gate dielectrics, in the interfacial region, at the Si-substrate/oxide interface and in Si. The gate dielectrics used in current industry are silicon dioxide (SiO_2) or silicon oxynitride (SiO_xN_y). Both donor-like and acceptor-like traps can be created in these dielectrics. According to the phenomenon of threshold voltage shift in the negative direction, we conclude that interface traps generated during NBTI are donor-like. Although a number of atomic mechanisms have been proposed, the exact mechanism of the defects generation is still in debate.

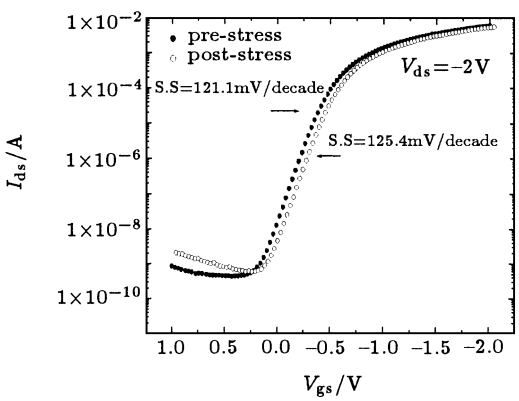


Fig.5. Comparison of I_{ds}-V_{gs} curve pre- and post-NBT stress with V_{g}=–2.75V at 100°C for 10000s.

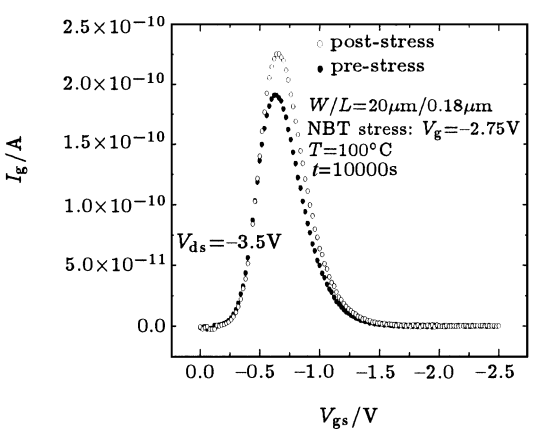


Fig.6. Change of gate current pre- and post- NBT stress with V_{g}=–2.75V at 100°C for 10000s.

3.2. The role of hydrogen

The presence of hydrogen has long been thought to be critical for NBTI in many reports,[1,2,4–11] and the presence of hydrogen is inevitable during device fabrication. Devices with SiO_2 gate oxide are

subjected to a post-processing anneal in hydrogen-containing forming gas to minimize the density of electronically active defects. Cracking centres are assumed to produce atomic hydrogen, which then passivates interface Si dangling bond species such as P_b centres and E'-type defects in bulk SiO_2. The passivated interfacial Si-H bond is the most typical precursor for interface traps. Under some stress conditions the removal of H atoms leads to dangling bonds which can capture carriers.

It has been proved that annealing the devices in deuterium ambient instead of hydrogen can significantly reduce the NBTI effect sensitivity. Due to deuterium's heavier mass or giant isotope effect, SiD bonds are more resistant than SiH bonds to hot carrier stress as well as NBTI. NBTI degradation with deuterium passivation generally exhibits a parallel shift compared to hydrogen passivation with a similar $t^{0.25}$ dependence, due to the lower diffusion coefficient of deuterium. This proves that hydrogen plays a major role during NBT stress. Hydrogen can exist in its atomic state H^0, as molecular H_2, as positively charged hydrogen or proton H^+, as part of the hydroxyl group OH, as hydronium, H_3O^+, or as hydroxide ions OH^-. Nowadays the research about hydrogen during NBTI is focused on its charge states, i.e. positively charged in the form of proton and neutral in the form of molecular H_2 or atomic H^0.

3.2.1. The charge states of diffusion species

First and foremost, the charge states of hydrogen during NBT stress should be identified, in general it is considered as in the form of positive charged proton[11,12] or neutral states such as atomic H^0 or molecular H_2.[5,6,9] According to the model of NBTI mentioned above in Eqs.(1) and (2), this is a diffusion controlled process. So for neutral diffusion species, the electric field has no effect on its transport. Thus, the diffusion rate is given by the ordinary diffusion equation:[5]

$$\frac{\partial C_X(x,t)}{\partial t} = D_X \frac{\partial^2 C_X(x,t)}{\partial x^2}, \tag{3}$$

where $C_X(x,t)$ is the concentration of X. On the other hand, for charged diffusion species, the external field strongly affects the transport of the diffusion species. In this case, the diffusion of charged species in an external electric field E_{ox} is described by the following equation:

$$\frac{\partial C_X(x,t)}{\partial t} = D_X \frac{\partial^2 C_X(x,t)}{\partial x^2} \pm \mu E_{ox} \frac{\partial C_X(x,t)}{\partial t}, \tag{4}$$

where μ is the mobility of the positively charged diffuser in the oxide. The plus sign corresponds to drift diffusion under positive bias temperature (+BT) stress, and the negative sign to that under negative bias temperature (-BT) stress. After removing the interface traps generation from hydrogen species, it may be expressed by the detailed balance equation:

$$\frac{\partial N_{it}(t)}{\partial t} = G[N_D - N_{it}(t)] - S[N_{it}(t)]^{1/a}[C_{xi}(t)]^{1/b}, \tag{5}$$

where $N_{it}(t) = [Si_3 \equiv Si^{\cdot}]$ is the concentration of the interface traps, $N_D = [Si_3 \equiv Si - H]$ is the initial concentration of interface defects, $C_{xi}(t)$ is the concentration of diffusing species X at the interface, G and S are field-dependent rate constants, and the exponent a and b are related to the reaction coefficient, which are determined by the details of the reaction. Here, [ ] indicates the concentration. The first term on the right side of Eq.(5) comes from the dissociation of $Si_3 \equiv$Si-H into $Si_3 \equiv Si^{\cdot}$, and the second term comes from the competing passivation of $Si_3 \equiv Si^{\cdot}$ by releasing hydrogen-related species, which has a suppressing effect. For the reactions occurring in the solid state phases, such as Si-substrate/oxide interface, the solution is difficult to derive, and for the ultrathin oxide the geometrical boundary conditions must be taken into account, which makes the mathematics more complicated. Ogawa *et al*[5,6] examined the time dependence of different charged diffusing species (H^0, H^+). Based on their solutions of the above equations under different boundary conditions, they concluded the primary degradation mechanism was dominated by diffusion of neutral species.

Another evidence for diffusion species not being positive charged is shown in Fig.8. On removing NBT stress, the PBT stress was applied to the device. PBT stress can recover a fraction of NBTI induced degradation as shown in Fig.7. After 10000s PBT stress the recovery of V_{th} can reach 25.42%, it shows that the degradation induced by NBTI consists of two parts: retrievable degradation and permanent degradation. Replotting this PBT recovery curve in log–log scale as shown in Fig.8, there is a break-off from the initial trend and drastic decrease at long stress time. So we can conclude that the diffusion species are neutral, for positive charged protons it should have the reverse behaviours under different gate voltage polarities, this means it should be time dependent with exponent of –0.25, but experimental results are not like that. Of the two possible forms of neutral hydrogen species (H^0

and H_2), it has been shown by many researchers that H^0 is unstable in the bulk. So H_2 is the most possible diffusion specie.

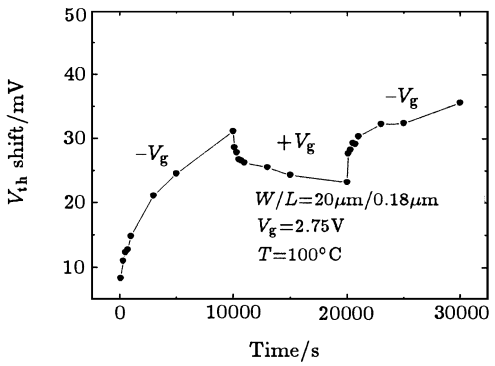


Fig.7. V_{th} shift of pMOSFET under NBT-PBT-NBT stress with V_g=–2.75V, 2.75V and –2.75V respectively at 100°C.

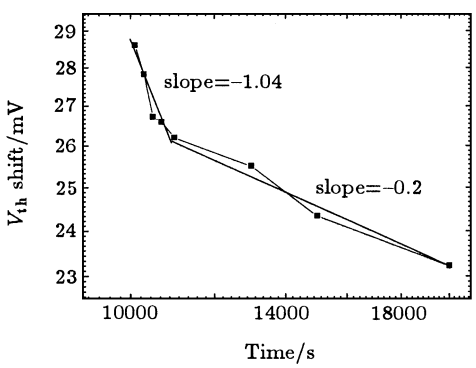


Fig.8. Replot of V_{th} shift under PBT stress with V_g=2.75V at 100°C in Fig.7 in log-log scale.

3.2.2. The migration of diffusion specie

The diffusion specie generated at the Si-substrate / oxide interface can migrate into oxide stack or silicon substrate, but in most reports only the direction towards gate oxide is considered.[1,4–6] Chakravarthi *et al*[7] compared the two-sided and one-sided diffusion processes by numerical simulations, they found the two cases predict identical time dependence. For mobile species generated at the Si-substrate / oxide interface, they can migrate towards gate oxide and Si-substrate direction. Threshold voltage can be simply expressed as follows:

$$V_T = V_{FB} - 2\phi_F - |Q_B|/C_{OX}, \tag{6}$$

where

$$\phi_F = (kT/q)\ln(N_D/n_i),$$

$$|Q_B| = (4qK_S\varepsilon_0\phi_F N_D)^{1/2}$$

and C_{ox} is the oxide capacitance per unit area. The flatband voltage V_{FB} is given by

$$V_{FB} = \phi_{MS} - \frac{Q_f}{C_{OX}} - \frac{Q_{it}(\phi_S)}{C_{OX}}, \tag{7}$$

where Q_f is the fixed charge density, Q_{it} is the interface trap density. It is always assumed that neither substrate doping density N_D nor oxide thickness vary with NBT stress.[1] But this may not be true if the hydrogen diffusion towards Si-substrate direction is considered. The charge state of isolated H within Si is an important issue because of its influence on migration and equally significant, its effects on the rate of trapping reactions with charged dopants.[13] It is now evident that H can exist in Si as an amphoteric center with positive, neutral, and possibly negative charge states. The distribution of H in these states, and hence its diffusion rate and reactivity, should depend on the position of the Fermi level. Hydrogen states in semiconductor exhibit great variety and complexity, largely due to the directional covalent bonding, the existence of several charge states and a comprehensive understanding is far from realization.[13,14] At least two-sided diffusion can increase degradation speed and result in more defects generation than one-sided diffusion. So the hydrogen two-sided diffusion must be taken into account as illustrated in Fig.9.

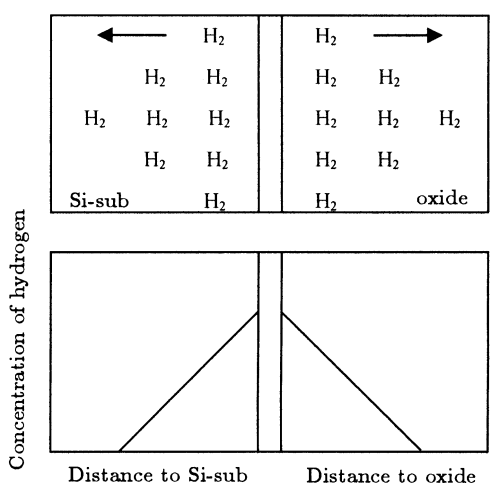


Fig.9. Illustration of hydrogen two sided diffusion.

4. Conclusion

NBTI has become an important reliability issue in pMOSFETs, it results in significant V_{th} shift and great drain current degradation, which becomes more severe as gate oxide is thinned down. However its exact mechanism is not still fully understood. By analysing the shift of pMOSFET parameters under NBT stress,

it was found that of all device parameters $V_{\rm th}$ has the largest shift and this shift can be partly recovered. However, this recovery is unstable and the degradation reappears after reapplication of NBT stress, which is primarily due to the depassivation and repassivation of donor-like interface traps, and these interface traps are closely related to the hydrogen passivated Si dangling bonds and its subsequently migration. Hydrogen species play a key role during device's NBT degradation, and they can present in the neutral or charged states. Both solutions of diffusion-drift equations and experimental results show that the diffusion species are neutral, and their subsequent migration is also important. In addition to diffusion towards gate oxide, hydrogen diffusion in the Si-substrate direction must be taken into account. Its transportation towards the Si-substrate and interaction with the dopants also has important influence on device degradation during NBT stress.

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