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# Impact of Initial Traps on TDDB and NBTI Reliabilities in High-k Gate Dielectrics

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## 1. Introduction

It has been well-known that high-k materials have a significant amount of initial traps contributing to a large initial leakage current. Hence, many efforts have been performed to suppress them. In contrast, the impact of such initial traps on various reliability issues has not been well studied, while we have proposed the generated subordinate carrier injection (GSCI) model[1] as the breakdown mechanism. Therefore, the purpose of this paper is to clarify the impact of initial traps in high-k gate dielectrics on the TDDB and NBTI reliabilities.

## 2. Experimental

$P^+$ poly-Si gated p-channel MOSFETs with $HfO_2/SiO_2$ gate dielectrics were fabricated on (100)Si. $HfO_2$ films were deposited on thermal $SiO_2$ layers by the following two methods to realize different initial trap densities with identical EOT: the ALD and the LL-D&A (layer-by-layer deposition and annealing)[2]. EOTs are 2.02 and 2.07 nm, and carbon contents in $HfO_2$ layers are $8.0x10^{14}$ and $7.4x10^{13}$ atom/cm$^2$ for ALD and LL-D&A samples, respectively. $HfAlO_X/SiO_2$ films with poly-Si and TaN gates were also evaluated.

## 3. Results and Discussion

*A. Impact of Initial Traps on TDDB Reliability*

Current-voltage (I-V) characteristics under positive polarity of $HfO_2/SiO_2$ films in ALD and LL-D&A samples are plotted in Fig.1. In low gate voltage ($V_G$) region, the ALD sample has larger current than the LL-D&A sample in spite of similar EOTs. We consider this difference is due to larger carbon content in $HfO_2$ layer of ALD sample[2]. Also under negative polarity, similar difference is observed as shown in Fig.2 plotted for hole current ($I_{hole}$). As indicated for LL-D&A sample, $I_{hole}$ can be divided into two components[1], $I_{DC}$ and $I_{TA}$. $I_{TA}$ is the trap-assisted current and is dominant in low $V_G$ region. $I_{DC}$, which is dominant in high $V_G$ region, is presumed in the GSCI model that the breakdown occurs when the fluence of $I_{DC}$ reaches the threshold[1]. In addition, $I_{DC}$ has a universal relationship to $V_G$[3] as plotted by broken curve in Fig.2. Therefore, the similar $I_{hole}$ in both samples in high $V_G$ region shown in Fig.1 suggests similar TDDB lifetimes, $T_{BD}$, under positive polarity. In fact, both samples have similar lifetimes under both polarities as shown in Fig.3. Thus, initial traps which induce large initial leakage do not impact on the TDDB reliability. This result is consistent with our previous work[4] on the effect of initial traps on the trap generation kinetics. Although $I_{DC}$ in ALD sample shown in Fig.2 is not clear due to large $I_{TA}$, the identical TDDB indicates that ALD sample has similar $I_{DC}$ to LL-D&A sample.

*B. Impact of Initial Traps on NBTI Reliability*

Fig.4 shows the stress time dependence of $\Delta V_{th}$ under NBT stresses in ALD sample, and Fig.5 shows the stress-$V_G$ dependence of $\Delta V_{th}$ after 1000s-stress in ALD and LL-D&A samples. Turn-around of $\Delta V_{th}$ to the stress-$V_G$ is clearly observed as was reported in [5]: $V_{th}$ shifts to *positive* in low stress-$V_G$ region and shifts to *negative* in high stress-$V_G$ region. *Negative* and *positive shifts* of $V_{th}$ are for and against well-known NBT degradation, respectively. ALD sample shows larger *negative shift* than LL-D&A sample as shown in Fig.5, while *positive shift* is in the similar level.

As shown in Fig.6, both samples exhibit similar $\Delta D_{it}$ with identical slopes. This result is consistent with the identical TDDB lifetimes of both samples shown in Fig.3, indicating similar trap generation rates. Therefore, the difference in the *negative shift* comes from the difference in the hole charging rate to the existing trap sites. When we express the discrepancies in $I_{hole}$ and in $\Delta V_{th}$ between ALD and LL-D&A samples by the discrepancy in $V_G$ ($\Delta V_G$) to obtain identical $I_{hole}$ and $\Delta V_{th}$, we find similar $\Delta V_G$ for $I_{hole}$ and $\Delta V_{th}$ (~1.8V in Fig.2 and ~1.6V in Fig.5). We obtained similar result also in another sample set of $HfAlO_X/SiO_2$ films deposited by both methods. Thus, it is concluded that initial traps strongly impact on the NBTI reliability by enhancing the charging current as well as by acting as charging sites.

In Fig.7, $\Delta V_{th}$ after 1000s-stress are plotted in relatively low stress-$V_G$ region for TaN and poly-Si gated various samples. In TaN gated sample ($HfAlO_X$, LL-D&A), only the *negative shift* is observed, while only the *positive shift* is observed in poly-Si gated samples ($HfO_2$ and $HfAlO_X$, ALD and LL-D&A). The *positive shift* is independent of the high-k layer ($HfAlO_X$ or $HfO_2$), initial trap density, and EOT. Despite of opposite directions of $V_{th}$ shift, both *shifts* in Fig.7 have similar stress-$V_G$ and stress time dependences each other when plotted by $|\Delta V_{th}|$ as shown in Fig.8 and Fig.9, respectively. In addition, the slope of $|\Delta V_{th}|$ to the stress time is 0.20~0.24 and is consistent with that of $\Delta D_{it}$ of 0.18~0.23.

Based on these results, it is possible to assume that trap species generated in TaN gated and poly-Si gated samples are not different, but just the dominant carrier types captured into such traps are different. While the mechanism explaining the later assumption is not clear, it seems plausible to expect the relationship between the *positive shift* and the Fermi-level pinning (FLP)[6], because of the lack of *positive shift* in TaN gated sample. This is consistent with reports on the effect of metal[5] and SiN-cap[7] insertions between poly-Si and HfSiON layers on the NBTI reliability.

## 4. Conclusion

Impact of initial traps in high-k gate dielectrics on the TDDB and NBTI reliabilities has been studied. Initial traps do not impact on the TDDB reliability as expected by the GSCI model. In the NBTI reliability, two mechanisms that induce *negative* and *positive shifts* of $V_{th}$ coexist in poly-Si gated samples, and initial traps degrade only the former one by increasing the hole charging into the existing trap sites. The *positive shift* is independent of the initial trap density and EOT, and has similar stress voltage and stress time dependences to the *negative shift* observed in TaN gated sample.

**Acknowledgment**

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**References**

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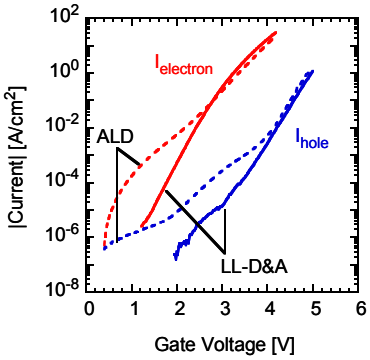


**Fig. 1** Current-voltage (I-V) characteristics of electron ($I_{electron}$) and hole ($I_{hole}$) currents of $HfO_2/SiO_2$ films in ALD and LL-D&A samples under positive gate voltages ($V_G$) measured by the carrier separation method.

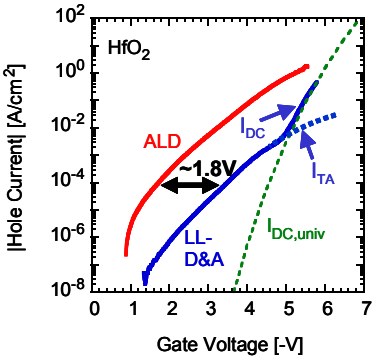


**Fig. 2** I-V characteristics of $I_{hole}$ under negative $V_G$. Two components consisting $I_{hole}$ of LL-D&A sample, $I_{DC}$ and $I_{TA}$, are indicated. Broken curve shows the fitted $I_{DC,univ}$ curve[3] to the measured $I_{DC}$. In ALD sample, $I_{DC}$ is not observable due to large $I_{TA}$.

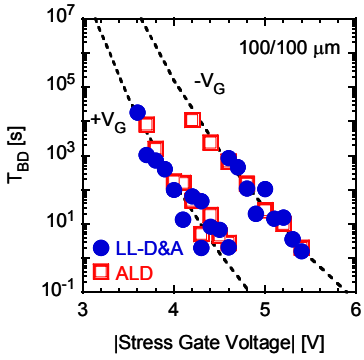


**Fig. 3** Measured TDDB lifetime ($T_{BD}$) of ALD and LL-D&A samples under both stress polarities plotted as a function of stress-$V_G$. Broken curves show the universal $T_{BD}$ curves[3] fitted to measured $T_{BD}$.

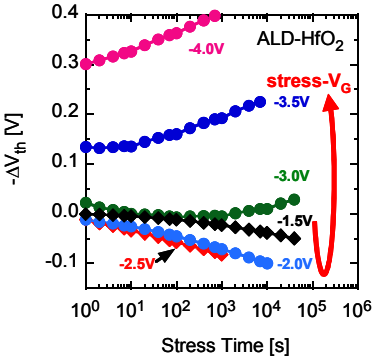


**Fig. 4** Stress time dependence of $\Delta V_{th}$ under NBT-stress with various stress-$V_G$ in ALD sample. Measurements were performed with p-ch MOSFETs (W/L=100/10 µm) at 120 °C.

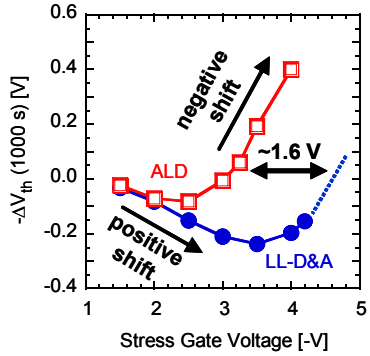


**Fig. 5** $\Delta V_{th}$ after 1000s NBT-stress in ALD and LL-D&A samples as a function of stress-$V_G$. Turn-around effect, *positive* and *negative shifts* in low and high stress-$V_G$ regions, is observed.

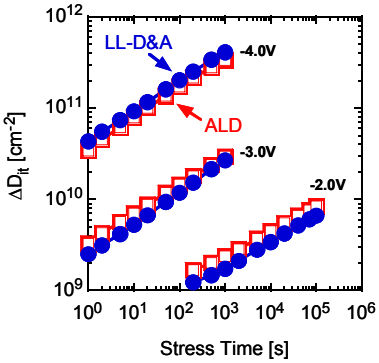


**Fig.6** Stress time dependence of the increment of interface state density, $\Delta D_{it}$, under NBT-stress in ALD and LL-D&A samples. $\Delta D_{it}$ were measured by the charge pumping method. Both samples show similar $\Delta D_{it}$ and slopes.

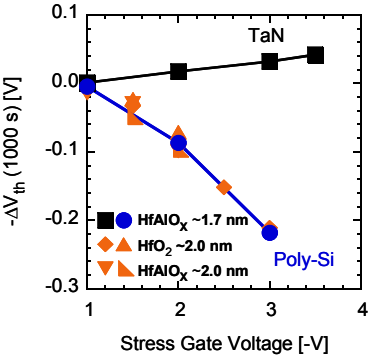


**Fig. 7** $\Delta V_{th}$ after 1000s NBT-stress in TaN gated sample and poly-Si gated samples plotted as a function of stress-$V_G$. *Positive shift* is not observed in TaN gated sample. All poly-Si gated samples show similar $\Delta V_{th}$ in this stress-$V_G$ region.

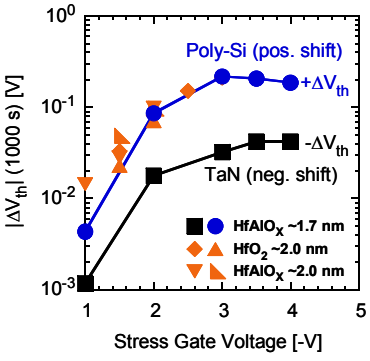


**Fig.8** $|\Delta V_{th}|$ after 1000s NBT-stress in TaN gated sample and poly-Si gated samples plotted in log-linear scale. *Positive* and *negative shifts* have similar stress-$V_G$ dependences each other.

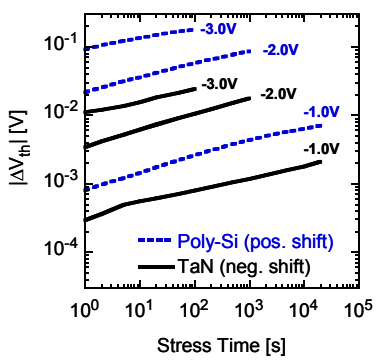


**Fig. 9** Stress time dependence of $|\Delta V_{th}|$ under NBT-stress of various stress-$V_G$ in poly-Si and TaN gated samples. *Positive* and *negative shifts* have similar slopes. The slope is similar also to that of $\Delta D_{it}$ in these samples (not shown).

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