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Evolution of Electron Trapping under Positive-Bias Temperature Stressing of the HfO_2/TiN Gate n-MOSFET

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I. Introduction

With the adoption of Hf-based high-*k* dielectrics for sub-45 nm CMOS technology, PBTI has become a serious reliability issue for the n-MOSFET [1], [2]. Studies have shown that electron trapping in the high-k layer is the main reason for the observed threshold voltage shift (ΔV_t) [3], [4]. Just like NBTI recovery [5], PBTI recovery also exhibits a logarithmic time dependence which spans many orders of magnitude [6]-[8], implying a broad spectrum of electron trap energies. In this work, we examine the evolution of ΔV_t under repeated stressing and relaxation. Under a relatively low oxide stress field (~5 MV/cm), the recovery of ΔV_t per cycle is observed to be a constant, independent of the number of times the device was stressed and relaxed, similar to the case of NBTI [9], [10]. However, at higher oxide stress fields (~7 MV/cm and above), the recovery of ΔV_t is observed to decrease with increase in the number of stress/relax (s/r) cycles. The decrease is found to occur in conjunction with an additional increase of deep-level electron trapping. The results imply that pre-existing shallow electron traps are being transformed into deeper ones by the high oxide stress field. Implications of this finding are briefly discussed.

II. Experimental Details

The gate stack of the n-MOSFETs studied consists of a 3 nm ALD HfO_2 on top of a 1 nm SiO_x interfacial layer. The metal gate is TiN. The EOT is 1.4 nm, as determined from capacitance measurement. Devices were subjected to 30 repeated s/r cycles. Each stress and relax phase lasted 1×10^3 s (i.e. the duty factor is 50 %). The temperature was fixed at 100 °C. Three different oxide stress fields were examined: a) 5.5 MV/cm; b) 7 MV/cm; c) 8.5 MV/cm. Relaxation was performed at a gate voltage (V_g) of either 0 or −1 V. The ultra-fast switching method, with a current resolution of 1 µA and a very short time delay of 100 ns, was employed for transfer curve measurement at certain time intervals [11]. ΔV_t was extracted by the constant subthreshold current (15 µA) method. Gate current (I_g) measurement was also performed to monitor bulk trap generation.

III. Results and Discussion

As depicted in Fig. 1, the recovery of ΔV_t is sensitive to the polarity of V_g, just like the case of NBTI [12]. After the first couple of hundreds of seconds under V_g = 0 V, the recovery is seen to slow down significantly and *appear* to saturate. But switching V_g to −1 V triggers another abrupt recovery of ΔV_t (Fig. 1(a)) If, however, the relaxation is first carried out with V_g = −1 V, a larger recovery is obtained and switching V_g to 0 V later has no impact on the subsequent ΔV_t recovery (Fig. 1(b)). The dependence of ΔV_t recovery on the V_g polarity and the order by which the negative V_g is applied imply the presence of deep-level electron traps. As illustrated schematically in Fig. 2(a), an electron trapped at a deep oxide trap could not readily detrap under V_g = 0, since it is confined by the filled valence band of the metal gate and Si substrate. On the other hand, when the trap level is raised above the Si valence band edge under a negative V_g, the trapped electron can be emitted spontaneously. It is to be noted that the remnant ΔV_t after the −1 V relaxation is on average only a couple of millivolts. This implies minor interface degradation under PBTI [13].

Fig. 3 shows ΔV_t fluctuation under repeated stressing and relaxation. To facilitate later discussion, the ΔV_t recovery in a given cycle is denoted as R and is given by the difference between ΔV_t at the end of the relax phase (ΔV_t^{eor}) and ΔV_t at the end of the preceding stress phase (ΔV_t^{eos}). ΔV_t^{eor} denotes the part of ΔV_t which did not recover at the end of the relax phase. The evolution of R (@V_g = 0) as a function of the number of s/r cycles is examined in Fig. 4. Under a low oxide stress field (5.5 MV/cm), R is constant regardless of the number of times the device was stressed and relaxed. Such a behavior is also seen under dynamic NBTI [9], [10]. The result implies that it is always the same group of oxide traps which are charged and discharged, respectively, under a given stress and relax condition. Interestingly, however, a gradual decrease of R is observed when the oxide stress field is increased.

To probe the reduction in R, we examine the increase in ΔV_t^{eos} or $\delta\Delta V_t^{eos}$, and the increase in ΔV_t^{eor} or $\delta\Delta V_t^{eor}$, measured with respect to the ΔV_t^{eos} and ΔV_t^{eor} of the first s/r cycle, respectively, as a function of the number of s/r cycles in Fig. 5. The rate of $\delta\Delta V_t^{eos}$ increase is comparable for the three oxide stress fields. However, the rate of $\delta\Delta V_t^{eor}$ increase is significantly higher for the case of the 7 and 8.5 MV/cm stresses, relative to that for the 5.5 MV/cm stress. It should be mentioned that ΔV_t^{eos} probes the effect of total electron trapping and interface state generation whereas ΔV_t^{eor} probes only the effect of remnant trapped electrons and interface state generation. A comparable rate of ΔV_t^{eos} increase means that the much higher rate of ΔV_t^{eor} increase at larger oxide stress fields is not a result of a greater interface state generation. The result shows that the decrease of R under a high oxide stress field is due to a faster increase of ΔV_t^{eor} relative to ΔV_t^{eos}, i.e. *a portion of the previously recoverable DV_t or electron trapping has been rendered more permanent as stressing progresses*.

We also examine the evolution of R (@V_g = −1 V) as a function of the number of s/r cycles in Fig. 6. The R in this case is larger than that of the 0 V relaxation, since deep-level electron traps are detrapped as well (cf. Fig. 1(b)). More importantly, the reduction of R is suppressed. For the 7 MV/cm stress, R is in fact constant, as opposed to the decrease observed under the 0 V relaxation. For the 8.5 MV/cm stress, the decrease in R is ~8 mV after 30 s/r cycles, as compared to the 21 mV decrease seen under the 0 V relaxation. This result shows that the reduction in R is due to shallower electron traps being transformed into deeper ones at high oxide stress field. Under 0 V relaxation, ΔV_t recovery or R is reduced due to the increase in the proportion of deep-level electron traps. A negative V_g helps the discharge of some of the deep-level electron traps, thus suppressing the decrease of R. For the 5.5 MV/cm stress, the R for both the 0 V and −1 V relaxation are constant, i.e. the proportion of shallow and deep-level electron traps does not change significantly over the period examined. This result means that the transformation from shallow to deep-level electron trapping is more likely to occur at higher oxide stress field.

The possibility of bulk trap generation under high oxide stress field was also examined by comparing the I_g versus V_g characteristics before and after PBTI stress. No apparent increase of I_g can be seen over the range of oxide stress field studied, implying that there is no generation of additional bulk traps (Fig. 7). It may thus be inferred that the decrease of R or increase in deep level electron trapping stems mainly from pre-existing shallow electron traps. At present, the mechanism for the increase in deep-level electron trapping is unclear as the atomic origin of the defect is not yet established. An interim explanation may be based on the oxygen vacancy V_O defect, which is a major source of electronic traps in the HfO_2. First-principles simulation has shown that V_O undergoes substantial structural relaxation when it captures an electron [14], due to the ionic nature of the HfO_2. A high oxide field could further facilitate such structural relaxation. The resultant reduction in system energy may over compensate the increase of the Coulomic energy (due to the electron capture), leading to a lowering of the trap level, as depicted schematically in Fig. 1(c). Since further scaling of the gate stack would increase the oxide field, the possible decrease of R and the corresponding faster rise in the more permanent ΔV_t may pose a challenge to the reliability of HfO_2 gate n-MOSFETs.

IV. Summary

This study shows that PBTI recovery is affected by the oxide stress field applied. Under a relatively low oxide stress field (~5 MV/cm), a constant recovery is observed, independent of the number of times the n-MOSFET was stressed and relaxed. At higher oxide stress fields, however, recovery is gradually reduced. Analyses involving negative gate recovery imply that the reduction in recovery is due to a part of the previously recoverable shallow electron traps being transformed into deeper level electron traps by the increased oxide field.

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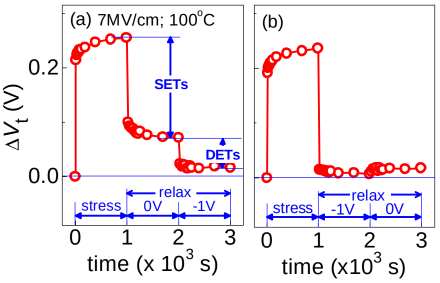

Fig. 1: (a) After PBTI stress, a large portion of the n-MOSFET degradation can be recovered with a 0 V gate voltage. This recovery is due to electron detrapping from shallow electron traps (SETs). An abrupt and substantial ΔV_t recovery can still be observed with a –1 V gate voltage applied after the 1000 s 0 V recovery. This recovery may be ascribed to electron detrapping from deep electron traps (DETs). (b) An initial –1 V gate voltage resulted in a near complete electron detrapping.

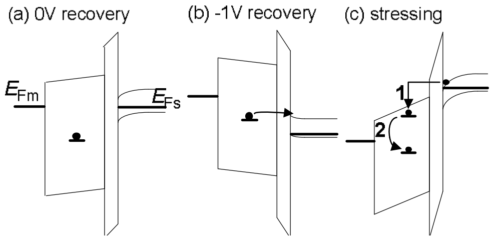

Fig. 2: Schematic energy band diagrams of a HfO_2 /TiN gate stack under different gate biasing: (a) An electron trapped at a deep oxide trap is confined by the filled valence band of the metal and p-Si and does not readily detrap under a 0 V gate voltage; (b) a negative gate voltage may facilitate the emission of the trapped electron by raising the trap level above the Si valence band edge; (c) an electron which tunnels from the Si conduction band into the HfO_2 conduction band is scattered and first captured by a relatively shallow oxide trap (arrow 1); subsequent structural relaxation may compensate the increase in Coulombic energy and lead to a lowering of the trap energy (arrow 2).

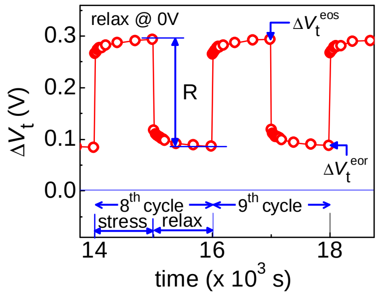

Fig. 3: Typical fluctuation of threshold voltage shift ΔV_t under dynamic PBTI. R is the portion of ΔV_t that recovered in the relax phase and is given by the difference between ΔV_t^{eos} and ΔV_t^{eor}, the respective ΔV_t at the end of the stress and relax phase. The component of ΔV_t which did not recover at the end of the relax phase is denoted by ΔV_t^{eor}.

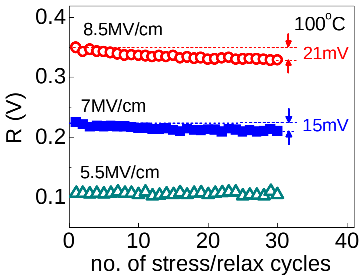

Fig. 4: The evolution of R (cf. Fig. 3) as a function of the number of stress/relax cycles under various oxide stress fields at a given temperature of 100 °C. R is constant at 5.5 MV/cm but shows a progressive decrease at higher oxide stress fields.

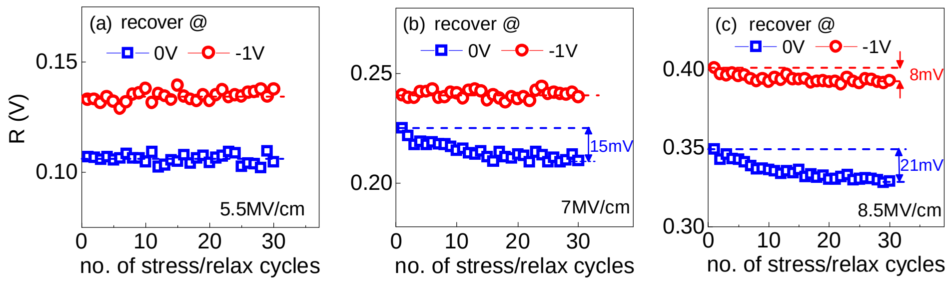

Fig. 6: The effect of a –1 V gate recovery voltage on p-MOSFETs stressed at (a) 5.5 MV/cm; (b) 7 MV/cm and (c) 8.5 MV/cm. The amount of R decrease (relative to the first cycle) is clearly suppressed for the latter two cases, as compared to the 0 V recovery. The R for the 7 MV/cm oxide stress field is in fact constant, just like the case of the 5.5 MV/cm stress field.

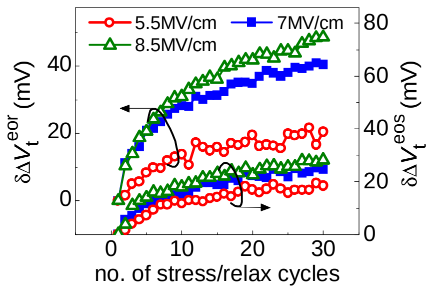

Fig. 5: The increase in ΔV_t^{eos}, with respect to the ΔV_t^{eos} of the first stress/relax cycle (denoted as $\delta\Delta V_t^{eos}$), are comparable for the three cases but the increase in ΔV_t^{eor}, with respect to the ΔV_t^{eor} of the first stress/relax cycle (denoted as $\delta\Delta V_t^{eor}$) is much larger for the 7 and 8.5 MV/cm oxide stress field as compared to that of the 5 MV/cm oxide stress field. This indicates that the decrease in R at higher oxide stress fields is due to a part of R being transformed into more permanent ΔV_t.

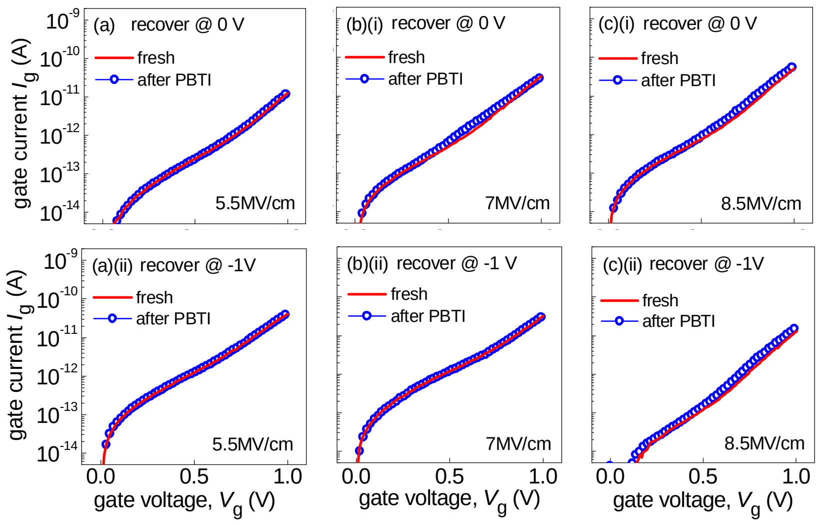

Fig. 7: No apparent increase of the gate leakage current after 30 cycles of dynamic PBTI is observed This indicates the absence of any significant generation of bulk traps in the HfO_2 gate stack over the range of oxide stress field examined. The results also imply that the reduction of R or increase of the relatively permanent ΔV_t observed in Figs. 4 and 5 involves the transformation of pre-existing shallow electron traps into deeper ones by the applied oxide stress field.