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On the Evolution of Switching Oxide Traps under Positive- and Negative-Bias Temperature Stressing of the HfO_2/TiN Gate Stack

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Motivation: Bias temperature instability (BTI) is one of the key reliability issues for the high-k/metal-gate stack. Recent work[1,2] has shown cyclical fluctuation of threshold voltage (V_t) under dynamic gate stressing, implying that it is always the similar group of oxide traps with predetermined capture/ emission characteristics which respond under a given set of experimental conditions. The purpose of this paper is to highlight the similarities/differences of the evolution of these oxide traps under repeated negative- and positive-bias temperature stressing/relaxation. The differences suggest distinct atomic origins of PBTI and NBTI. Possible atomic models are proposed.

Experiment/Simulation: Test devices were n- and p-MOSFETs fabricated on the same wafer. The gate stacks consist of a 1-nm SiO_x interfacial layer and 3-nm atomic-layer-deposited HfO_2 and the metal gate is TiN. Both devices have very similar EOTs of ~1.4 nm. The ultra-fast switching method[3], with a very short delay of ~100 ns, was employed to measure the V_t shift during stress and relaxation. The devices were subjected to numerous repetitive stress and relaxation phases, each lasting 1×10^3 s. One dynamic BTI (DBTI) cycle comprises one stress phase and the following relaxation phase. The V_t recovery per cycle or R was examined as a function of the number of DBTI cycles (Fig. 1) to probe the impact of stressing on the oxide-trap characteristics. First-principles simulation of possible defect structures was carried out using VASP[4].

Similarities: (1) At low oxide stress field (~5 MV/cm), the R is constant, independent of the number of DBTI cycles, irrespective of whether it is PBTI or NBTI stress. The constant R may be explained in terms of trapping/detrapping response of a similar group of oxide traps under a given set of experimental conditions. (2) When the oxide stress field is increased, R decreases progressively with the number of DBTI cycles. As discussed previously[2,5], the decrease of R is due to a portion of the initially recoverable oxide traps being rendered more permanent as stressing progresses, i.e. the emission time constants of these oxide traps are gradually increased or trap levels are shifted deeper thus locking in the trapped charge. This is reflected in Fig. 2, which shows that the relatively permanent part of ΔV_t, i.e. the part which did not recover at the end of each recovery cycle, increasing more rapidly as compared to the total V_t shift[2,5].

Differences: (1) Relaxation experiments involving an opposite gate polarity (from that of stress) shows no influence on R decrease under NBTI stress (Fig. 3). On the other hand, the R decrease is almost entirely suppressed for PBTI stress. These results imply that the decrease of R for NBTI stress is irreversible whereas it is reversible for PBTI stress. (2) A substantial stress-induced leakage current (SILC) is observed when the R decreases under NBTI stress (Fig. 4). It should be mentioned that SILC is strongly correlated to R decrease[5], as in the case of the SiON p-MOSFET[6,7]. However, almost no SILC is observed when R decreases under PBTI stress.

Possible Defect Models: Although the evolution of R under PBTI and NBTI stresses is broadly similar, the differences observed under an opposite gate relaxation polarity and the different outcomes of SILC measurement imply that distinct oxide defects are involved. Many studies have shown that the oxygen vacancy (V_O) defect is a major source of hole traps in the HfO_2. When a hole is captured at V_O, structural relaxation (enhanced by the oxide field) would render these trapped-hole sites relatively permanent. Simulation has shown that the hole-trap levels are rather deep, ~4 eV from the HfO_2 valence band maximum (Fig. 4), making them excellent trap-assisted tunneling centers for electrons from the gate under a negative gate bias. On the other hand, V_O's are very shallow electron traps and therefore cannot explain the R decrease observed under PBTI. This latter behavior must necessarily involve much deeper electron traps. Our simulation study reveals the V_O-O_i (O_i denotes an interstitial O atom in the vicinity of V_O) defect pair as a possible candidate for a deep electron trap (>2.5 eV below the HfO_2 conduction band). Changes in the position of the O_i, induced by a high oxide stress field, could further shift the trap level downwards, locking in the trapped electron (not shown).

References: [1] Gao *et al.*, *Proc. IRPS*, 943 (2011); [2] Gao *et al.*, Proc. SSDM, 835 (2012);[3] Du *et al. IEEE EDL*, **30**, 275 (2009); [4] Kresse and Hafner, *Phys. Rev. B*, **47**, 558 (1993); [5] Gao *et al.*, *Proc. IRPS*, 5A.5.1 (2012) [6] Boo *et al.*, *IEEE EDL*, **33**, 486 (2012); [7] Boo *et al.*, *IEEE TED*, **59**, 3133 (2012).

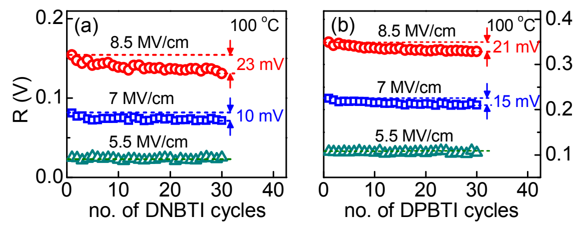

Fig. 1: The evolution of R (ΔV_t recovery per relaxation phase) during 30 dynamic (a) NBTI and (b) PBTI cycles.

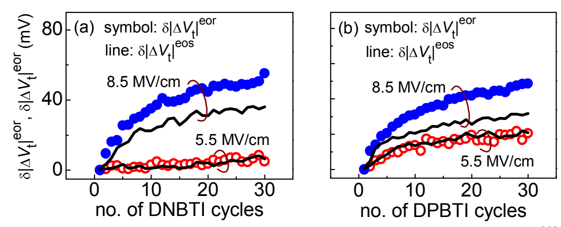

Fig. 2: Incremental change (measured w.r.t. the first cycle) of ΔV_t^{eos} (total ΔV_t shift at the end of every stress phase) and ΔV_t^{eor} (the part of ΔV_t shift which did not recover at the end of each relaxation phase) as a function of (a) DNBTI and (b) DPBTI cycles.

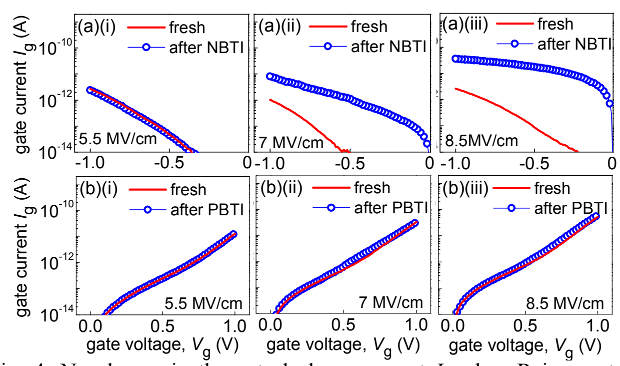

Fig. 4: No change in the gate leakage current I_g when R is constant under either NBTI or PBTI stress. A significant increase of I_g is observed when R decreases under NBTI stress. However, no apparent change in I_g is seen under PBTI when R decreases.

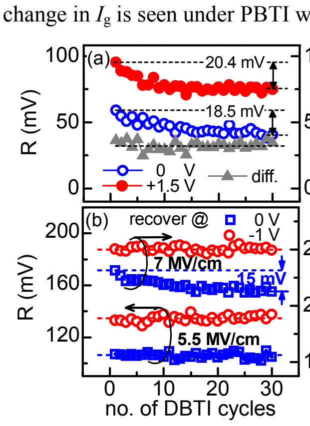

Fig. 3: (a) NBTI: Relaxation performed under a positive gate voltage has no apparent impact on the R decrease. (b) PBTI: A negative gate relaxation voltage suppresses the R decrease.

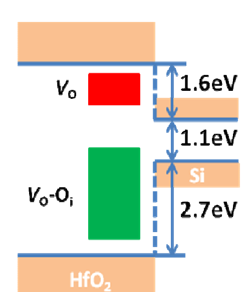

Fig. 5: Energy band diagram showing the range of trap energies for the V_O and V_O-Oi defects in the HfO_2 bandgap. Also shown are the band offsets with Si.