Bias-Temperature Instability in the High-k/Metal Gate Stacks

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Besides the negative-bias temperature (NBTI) effect that is seen in the conventional polysilicon on SiO₂ or SiON gate stack, the high-k/metal gate stack also exhibits positive-bias temperature instability (PBTI) which has an adverse impact on the operation of the n-MOSFET. Significant threshold-voltage $V_t$ shift but negligible transconductance $g_m$ degradation was observed after PBTI stress. On the other hand, both a substantial shift in $V_t$ and degradation of $g_m$ were observed after NBTI stress. On this basis, some studies have concluded that PBTI and NBTI are due to different physical mechanisms. The lack of interface degradation in the case of PBTI may be understood in terms of the absence of the PBTI effect in the SiO₂ dielectric. However, the role of charge trapping in the high-k dielectric remains poorly appreciated and is often viewed as resulting from the transient “filling/emptying” of pre-existing oxide defects which may not have any impact on long term device degradation.

In this talk, we will present experimental results from our recent dynamic BTI studies on the HfO₂/TiN gate stack. In terms of charge trapping and oxide defect generation in the high-k oxide, dynamic PBTI and NBTI exhibit both similar and different experimental features:

- **Similarity** – Hole trapping and electron trapping are observed to evolve gradually, when the test device is being “cycled” numerous times between stress and relaxation, from a transient state (i.e. the trapped charge could be re-emitted within the relaxation period chosen) into a more permanent state (i.e. the trapped charge could no longer be re-emitted within the relaxation period chosen). The observed evolution implies that the some of the trap levels might have shifted from shallow to deep, thus “locking” in the trapped charges. The result also implies that trap properties are continuously changing and may not be presumed as static and described by fixed capture/emission time constants.

- **Difference** – When part of the transient hole trapping is changed into a more permanent state, generation of stress induced leakage current (SILC) can be clearly observed. However, no SILC generation is observed in the case of the dynamic PBTI when part of the transient electron trapping has evolved into a more permanent form.

To probe the reason(s) behind the similarity and difference observed, ab-initio simulation was performed on an amorphous HfO₂ supercell using VASP, focusing first on the oxygen vacancy ($V_O$) defect, since this is the dominant source of oxide traps in high-k dielectrics. The supercell consists of 64 O atoms and 32 Hf atoms, allowing the properties of 64 different $V_O$ defects to be studied following charge capture and full structural relaxation. Simulation data reveals an average charge transition level (CTL) of $3.43 \pm 0.31$ eV for the neutral-to-positive charge state transition. This indicates that $V_O$’s in the HfO₂ could function as deep-level hole traps, accounting for the hole-trap transformation observed. On the other hand, the average CTL for the neutral-to-negative charge state transition is $4.44 \pm 0.12$ eV. This means that even after having gone through full relaxation following an electron capture, the $V_O$ defect remains as a very shallow electron trap and it could not explain the shallow-to-deep evolution of the electron traps observed experimentally.

Ab-initio simulation was performed to examine the physical properties of another related defect – the vacancy-interstitial ($V_O$-$O_i$) pair. We consider the $V_O$-$O_i$ as a likely candidate for the observed BTI effect given that high-k oxides are ionic and oxygen is relatively mobile in the high-k oxides. Depending on the position of the $O_i$ relative to $V_O$, simulation shows that the CTL has a broad energy distribution, ranging from slightly under the conduction band edge to slightly above the valence band edge of the HfO₂. This shows that the $V_O$-$O_i$ defect could function both as a very shallow and very deep trap in the HfO₂. The lack of SILC generation in the case of PBTI as opposed to the apparent SILC generation in the case of NBTI may be reconciled by treating the $V_O$-$O_i$ defect as an intermediary prior to the formation of the $V_O$ defect. For certain strategic positions of the $O_i$, it is shown that the $V_O$-$O_i$ defect could function as a deep electron trap (and thus does not participate in the trap assisted electron tunneling process) and at the same time as a relatively shallow hole trap that could give rise to the SILC in the case of NBTI.