TCAD Incorporation of Physical Framework to Model N and P BTI in MOSFETs

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Abstract: Negative and Positive Bias Temperature Instabilities (NBTI, PBTI) respectively in P and N channel High-K Metal Gate (HKMG) MOSFETs are modeled by trap generation (TG) and charge trapping (CT) and validated against measured data. The mechanism of TG (interface) is incorporated into TCAD and is separately validated using independent experiments. BTI kinetics is modeled at different stress bias (Vg) and temperature (T). Impacts of Nitrogen (N%) and Equivalent Oxide Thickness (EOT) scaling on the magnitude of BTI and its time, Vg and T dependencies are modeled.

Keywords: threshold voltage shift, DCIV, NBTI, PBTI, EOT scaling, HKMG-MOSFETs, Nitrogen impact

I. INTRODUCTION
Bias Temperature Instability (BTI) is a crucial reliability issue in P and N channel HKMG MOSFETs [1]. It causes shift in several device parameters such as threshold voltage (ΔVt), linear (ΔIdLs) and saturation (ΔIsSat) drain current, subthreshold slope (ΔSS) and transconductance (Δgds) etc. over time, due to the buildup of positive charges in the gate insulator of the transistor. These parameters recover partially when the stress is lowered or removed, resulting in lower degradation during AC as compared to DC stress. The BTI mechanism is debated and various models are proposed [2]-[4]. It is now believed that ΔVt during NBTI in P MOSFETs is due to TG at the channel/interlayer (IL) interface (ΔVt_IL) and IL bulk (ΔVt_IL), and CT (hole, ΔVt_HK) in IL bulk, and ΔVt during PBTI in N MOSFETs is due to the TG at IL/HK interface (ΔVt_IL-HK) and HK bulk (ΔVt_HK), and CT (electron, ΔVt_HK) in HK bulk, see Fig.1 [1]. The BTI Analysis Tool (BAT) utilizes the uncorrelated contributions from the above subcomponents of overall ΔVt, Fig.2, and can model the ΔVt kinetics during DC and AC stress and recovery, as Vg, T, pulse duty cycle and frequency are varied for PBTI [5] and NBTI [6], [7], and various process changes for NBTI [7]. BAT uses double interface Reaction-Diffusion Model (RDM) for interfacial TG (density ΔNt_Il or ΔNt_HK), their charged state and contribution (ΔVt_IL or ΔVt_HK) by the Transient Trap Occupancy Model (TTOM) and empirical models for CT and bulk TG. Recently, the Activated Barrier Double Well Thermionic Model (ABDWTM) is used for hole CT for NBTI [8]. The interfacial TG kinetics during NBTI has been modeled using TCAD and validated using Direct-Current I-V (DCIV) data [12], [13]. The TCAD-NBTI framework utilizes Capture-Emission Depassivation Model (CEDM), Fig.3, and Multi-State Configuration Model (MSCM), Fig.4 to calculate TG kinetics. The framework is validated using FinFETs with different channel materials, see [9] for further details.

II. SCOPE OF WORK
PBTI interfacial trap generation is incorporated in TCAD and validated using DCIV. Although experiments suggest TG at the channel/interlayer and interlayer/High-K respectively for N and P BTI [1], due to the absence of coupling between non-local tunneling and CEDM at present, TG is calculated at the channel/IL interface for both cases, but generated traps are assigned at the IL/High-K interface to obtain ΔVt during PBTI. TG kinetics measured using DCIV method at various Vg and T, in N and P HKMG MOSFETs having different N% and IL thickness (data from [9]) is modeled by TCAD. ΔVt time kinetics measured using ultra-fast I-V method for the same devices [5], [6] is modeled using BAT, with the underlying interfacial TG component validated using TCAD. Impact of N% induced IL scaling (leading to EOT scaling) is modeled.

III. BTI MECHANISM
Inversion layer holes tunnel to Hydrogen (H) passivated defect precursors at the channel/IL interface at Vg<0V stress, react, break (=ΔNt_HK) and release H, Fig.3. The released H atoms diffuse and react with other H passivated defects inside IL (HK) bulk to form H2, which diffuses away, Fig.4. This is RDM for NBTI. Interfacial TG (from DCIV) shows similar power low time kinetics for both N and P BTI [1]. A similar process as RDM for NBTI is used for PBTI at Vg>0V stress, with inversion electrons induced dissociation of the defect precursors at the IL/HK interface (=ΔNt_HK). H atoms diffusion and defect generation at the HK bulk, and diffusion of H2 (Figs.3 and 4), which is RDM for PBTI. The chemical nature of defects is likely different for the interfacial TG in N and P BTI. ΔNt_HK can be created directly by electrons, or by the Anode Hole Injection (AHI) process, i.e., tunneling of electrons from cathode to anode, impact ionization and injection of energetic hole into gate oxide, although a direct link (the former) is used in TCAD at present. Moreover, the tunneling and trapping of holes (IL) and electrons (HK) result in CT, and AHII process is also responsible for bulk TG, and these effects are handled separately in BAT.

IV. TCAD FRAMEWORK
Two-dimensional P and N channel HKMG-MOSFET device structures are generated using process simulation [12]. In device simulation [13], defect dissociation by holes (NBTI) and electrons (PBTI) is handled using CEDM-MSC framework. Only four CEDM model parameters, i.e., the pre-factor (Kp0), temperature activation (Ea(Kp)), temperature (T) independent field acceleration (Γ0), and bond polarization (α),
Fig.3, are related to bond dissociation, and are varied to model different IL based devices used in this work. MSCM is used for diffusion of released H after bond dissociation using CEDM, dimerization into H₂ molecule assisted by reaction with another H passivated defect (at IL/High-K interface) and H₂ diffusion. All MSCM parameters are consistent between studied devices for N & P BTI. Backend of 1µm is used to allow H₂ diffusion in both BTI (length depends on stress time and T that determine the distance of H₂ diffusion).

V. DEVICE AND MEASUREMENT DETAILS
Gate First (GF) N and P HKMG MOSFETs having ultrathin thermal IL and HfO₂ HK are used [1]. IL scaling is done using thermal process tweak for D1 (5Å) and D2 (3Å), with N% in D₂ for D3 (2.5Å) and N based IL. D4 (1.5Å), EOT of HK is 4.6Å. DCIV measured data in Figs.5-8 and Figs.12-15 are with delay correction [11], and in Figs.12-15 with (also) bandgap correction (ΔV_T = K.ΔN_IT) [2]. ΔV_T in Figs.9-14 are measured with 10µs delay [5], [6].

VI. TCAD MODELING
Modeling of DCIV measured ΔN_IT time kinetics at various V₀ and T are shown for N, P BTI, for devices having various N% and IL, in Figs.5 and 6. Only longer time (>10s) data are available as DCIV is a slow method. Power law time kinetics is observed with n=1/6 for all cases (after delay correction), the slope is determined by H₂ diffusion and suggests similar process for the time kinetics in N, P BTI. Model accuracy is verified using data at different V₀ x T, Fig.7. ΔN_IT increases for NBTI but reduces for PBTI as N% is increased, Figs.5, 6, 8, due to their different origin. The Voltage Acceleration Factor (VAF, slopes in Fig.8) reduces at higher N% for both N and P BTI.

VII. BTI MODELING
Measured and modeled ΔV_T kinetics are shown for N and P BTI, Figs.9, 10. The underlying subcomponents (ΔV_T from RDM, ΔN_IT and ΔV_T from ABDWTM) are shown at fixed V₀, T, Fig.9. Interface TG dominates ΔV_T for both N, P BTI at longer time (>1s) and shows power-law time dependence with slope of n~1/6, due to H₂ diffusion in RDM as discussed before. DCIV calibrated TCAD with a fixed correction factor K is used for difference in scanned bandgap between DCIV and V_T measurements [2]. Bulk TG also has power-law time dependence with long-time slope n/1.3. CT saturates at long time (n~0 in a log-log plot). The model is validated across different V₀ and T, Fig.10, 11 (only few examples are shown, the validation is done for other stress conditions as well).

VIII. EOT SCALING
Modeling of measured overall ΔV_T (from ultra-fast I-V) and ΔV_T (from DCIV) versus EOT is shown in Fig.12. Time slope n, Fig.13, T activation energy (Eₐₜ), Fig.14 and VAF, Fig.15 versus EOT (~IL scaling) of ΔV_T and ΔV_T are shown for N and P BTI. ΔV_T dominates ΔV_T, both for NBTI and PBTI, in these experiments. There is a slight reduction in PBTI degradation at scaled EOT (due to Nitridation). This is consistent with higher N% resulting in higher ΔV_T of IL and lower ΔV_T (from calibrated TCAD), lower ΔV_T, and ΔV_T, and higher pre-existing trap density (it is verified by 1/f noise measurements in [1]). Since CT saturates, n of ΔV_T reduces at lower EOT (more reduction than n of ΔV_T, Figs.13. Since CT has lower E₂ than TG [5]-[8], E₂ of ΔV_T reduces (more reduction than ΔV_T) at lower EOT due to Nitridation (D3). VAF for ΔV_T hence ΔV_T reduces for both BTI as IL is scaled (as ΔV_T dominates ΔV_T), Fig.15.

IX. CONCLUSION
TCAD is enabled for interface TG during BTI in N and P channel MOSFETs. BAT with RDM for interface TG (same as TCAD) and ABDWTM for CT is used to model N and P BTI in differently processed MOSFETs. TCAD and BAT are separately validated with measured BTI data from differently processed devices. Further work is underway to incorporate a Reaction Drift Diffusion Model (RDM) for bulk TG and ABDWT for CT for complete BTI solution using TCAD.

REFERENCES
Fig.1. Schematic of the trap generation (TG) and trapping (CT) mechanism is shown under both NBTI and PBTI stress for a planar HKMG device.

Fig.2. Schematic of BAT framework for both NBTI and PBTI stress-recovery for a planar HKMG device. \( \Delta V_T \) subcomponents and corresponding models are shown.

Fig.3. Schematic of H passivated bond dissociation process at the channel/IL interface used in CEDM [9].

Fig.4. Multi State Configuration Model schematic, utilizing CEDM, showing Hydrogen Transport degradation mechanism at the two interfaces for N(h+) and P(e-) BTI.

Fig.5. TCAD modeling of DCIV measured \( \Delta N_{IT-IL} \) time kinetics showing increased NBTI degradation for (b) nitried device (D4) as compared to (a) non-nitried device (D2). Lines: TCAD simulation, symbols: DCIV data.

Fig.6. TCAD modeling of DCIV measured \( \Delta N_{IT-HK} \) time kinetics showing lower PBTI degradation for (b) nitried device (D4) as compared to (a) non-nitried device (D2). Lines: TCAD simulation, symbols: DCIV data.

Fig.7. TCAD modeling of field dependence of DCIV measured \( \Delta N_{IT-IL} \) for N (left), and \( \Delta N_{IT-HK} \) P(right) BTI for different IL scaled devices. Lines: TCAD simulation, symbols: DCIV data.

Fig.8. TCAD modeling of field dependence of DCIV measured TG, \( \Delta N_{IT-IL} \) for (left) N and \( \Delta N_{IT-HK} \) for (right) P BTI at different temperature. Lines: TCAD simulation, symbols: DCIV data.
Fig. 9. BAT modeling of ultra-fast measured $\Delta V_T$ and DCIV measured TG time kinetics for top: NBTI during (a) stress and (b) recovery; and bottom: PBTI during (c) stress and (d) recovery; at fixed $V_{G-STR}$ and the sub-components are shown. Overall $\Delta V_T$ is dominated by $\Delta V_{IT}$ subcomponent.

Fig. 10. BAT modeling of ultra-fast measured NBTI $\Delta V_T$ time kinetics for (a) stress and (b) recovery at different $V_{G-STR}$ are shown. Only few cases of $V_{G-STR}$ are shown for better visibility. Measured data: symbols, model data: lines.

Fig. 11. BAT modeling of ultra-fast measured NBTI $\Delta V_T$ time kinetics for (a) stress and (b) recovery at different $V_{G-STR}$ are shown. Only few cases of $V_{G-STR}$ are shown for better visibility. Measured data: symbols, model data: lines.

Fig. 12. Ultra-fast measured fixed time $\Delta V_T$ and TG from DCIV, NBTI (top), and PBTI (bottom); for different IL-scaled devices are modeled using BAT. Measured data: symbols, model data: lines.

Fig. 13. Time slope of ultra-fast measured $\Delta V_T$ and TG from DCIV, NBTI (top), and PBTI (bottom); for different IL-scaled devices are modeled using BAT. Measured data: symbols, model data: lines.

Fig. 14. Temperature Activation Energy ($E_A$) of ultra-fast measured $\Delta V_T$ and TG from DCIV, NBTI (top), and PBTI (bottom); for different IL-scaled devices are modeled using BAT. Measured data: symbols, model data: lines.

Fig. 15. Voltage Acceleration Factor (VAF) of ultra-fast measured $\Delta V_T$ and TG from DCIV, NBTI (top), and PBTI (bottom); for different IL-scaled devices are modeled using BAT. Measured data: symbols, model data: lines.