# Degradation Investigation of High-k/Metal Gate nMOSFETs by 3D KMC with Multiple Traps Interactions

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## Abstract

This paper investigates degradation behaviors in high-k/metal gate stack of nMOSFET with multiple traps interaction by 3D Kinetic Monte-Carlo (KMC) simulation method. The novel microscopic mechanisms are simultaneously considered in a compound system which includes: (1) trapping/detrapping from/to channel/gate; (2) trapping/detrapping to other traps (3) traps generation and recombination. Different type of traps distribution shows largely different behaviors of RTN and BTI.

## 1. Introduction

Reliability and variability of high-k oxide layer are mainly attributed to traps performance which induce random telegraphy noise (RTN), bias temperature instability (BTI) and trap-assisted-tunneling (TAT) [1]. Prospective high-k material, HfO<sub>x</sub> as gate oxide in MOSFETs also shows unstable under bias and thermal stress. Oxygen vacancy defects in HfO<sub>x</sub> can capture and emit electrons, which can induce RTN and BTI degradation. Meanwhile, new traps can be generated in HfO<sub>x</sub> under stress conditions [2,3]. Furthermore, electrons transferring between oxygen vacancy defects in high-k dielectric material can cause gate leakage current [4]. Models of RTN, BTI and TAT only considering trapping and detrapping from/to channel/gate cannot describe the chaotic multi-physical processes. Therefore, traps generation/recombination and trapping to/from other traps should be considered to analyze degradation behavior in high-k gate stack device.

In this work, a simulator is developed with consideration of traps interaction and traps generation/recombination by 3D KMC method. Characteristics of threshold shift and RTN are simulated. Traps distribution effects are explored and TAT path and critical traps are extracted.

## 2. Simulation Method and Device Structure

3D KMC method is applied in simulation with trapping/detrapping from/to channel/gate/other traps and traps generation and recombination as shown in Fig 1. Five microscopic mechanisms are fully coupled. Traps are coupled with each other due to the interaction. As a result, states of empty and filled in critical traps restrict activity of other near traps. Trapping/detrapping processes are well interpreted with nonradiative multiphonon transition models [5]. Traps generation and recombination are described by chemical reaction models [7].As shown in Fig. 2, the simulation results, dependence of capture and emission times of three traps on gate voltage (Vg), have excellent agreements with measurements [6]. It illustrates that capture time  $\tau_c$  decreases with Vg, while emission time  $\tau_e$  increases in Fig. 2.

n-channel MOSFETs with 5nm  $HfO_2$  stack are used in our simulation. The gate length is 25nm, which is equal to the width (W/L=25/25nm). Permittivity of  $HfO_2$  is 22. A constant voltage is applied on gate with source and drain ground. Multiple traps in high-k layer are considered during simulation.



Fig. 1 Multi-physical models including trap generation/ recombination, trapping (a) from/to channel (b) from/to other traps (c) from/to metal gate.



Fig. 2 Dependence of  $\tau_c$  (solid symbol) and  $\tau_e$  (opened symbol) on gate voltage Vg with three traps. The experimental results[6] is also plotted.

#### 3. Results and Discussion

Traps distribution (W=12.5nm) is shown in Fig. 3. High light points represent trap positions and bright degree is equivalent of activity degree that refers to statistical average trapping and detrapping times per second. Obviously, traps near channel are more active than ones far from channel in Fig. 3 (a), which indicates that traps far from channel can exchange electrons with near traps but hardly interaction with channel. As a result, activity degrees are determined by the near traps which are close to channel. However, after adding a trap #6 as shown in Fig. 3 (b), the distribution of activity degrees greatly change. Traps #3,#4 and trap #5 become more active than before, because trap #6 acts as a bridge connecting inside traps with metal gate, which promotes the flow of electrons. Meanwhile, a TAT path is generated in Fig. 3 (b). It can be concluded that inside traps in critical path actively contribute to TAT and RTN, while isolated traps have little involvement in TAT but can cause BTI.



Fig. 3 (a) Interaction path with 5 traps (b) transition path with 6 traps. High light points represent trap positions and bright degree is equivalent of activity degree that refers to statistical average trapping and detrapping times per second.



Fig. 4 Transient characteristics of  $\Delta V_{th}$  with (a) 5 traps and (b) 6 traps corresponding to Fig. 3. (black line: statistical averaged  $\Delta V_{th}$ , red/blue line: typical examples of transient  $\Delta V_{th}$ , gray line: 100 samples)



Fig. 5 (a) Transient characteristic of TAT currents with 6 traps corresponding to Fig. 3 under different gate voltage (b) Distribution of Statistical TAT current.

Fig. 4(a) and (b) show PBTI and RTN induced threshold voltage shifts  $\Delta V_{th}$  under two type distribution of traps corresponding to Fig. 3(a) and (b). In Fig. 4(a), it can be seen that without TAT path of trap #6,  $\Delta V_{th}$  rapidly reach to steady value and traps states tend to be stable. The rising step can be easily found with 5 traps. However, Fig. 4(b) shows large instability of  $\Delta V_{th}$  with TAT path of trap #6. Due to the interaction of traps and stable path of electrons flow, states of traps in critical path cannot keep invariant. More events of RTN occur in  $\Delta V_{th}$  and severe variability leads to decrease of statistical average  $\Delta V_{th}$ . Fig. 5 (a) presents that TAT currents with multiple traps interaction increase with Vg. It can be seen that TAT currents are sensitive to gate voltage under low stress and variability of TAT current is enlarged with  $V_{g}$ . Fig. 5 (b) shows variation of TAT current distribution with Vg.



Fig. 6 Degradation of threshold voltage with consideration of traps generation.

Fig.6(a) shows that count of traps grow with time under high gate bias and temperature stress. Fig.6(b) shows the degradation of threshold voltage. Traps distribution follows stochastic uniform and trap energy levels follow Gaussian distribution. Traps generation and recombination are considered in simulation. Stress induced new traps directly impact on transient characteristic of  $\Delta V_{th}$ .

## 4. Conclusions

Characteristics of PBTI, RTN and TAT current are explored by 3D KMC simulation with consideration of multiple traps interaction and traps generation/recombination. Traps distribution in HfO<sub>2</sub> stack greatly affects RTN, BTI and TAT current. TAT path and critical traps are extracted. Degradation of gate oxide layer under high stress is discussed. Details of degradation are well described with coupling multiple microscopic mechanisms.

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