3D KMC Reliability Simulation of Nano-Scaled HKMG nMOSFETs with Multiple Traps Coupling

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***Abstract*—This paper presents coupling characteristics of multiple traps in HKMG nMOSFETs by a 3D kinetic Monte-Carlo (KMC) simulator we developed, which includes several fully-coupled multi-physical models: trap generation/ recombination, trapping/detrapping to/from channel, metal gate, and the interaction of traps. It shows that activation energy and trapping/detrapping from/to channel/gate impact on coupling of multiple traps. Interaction of traps complicates mechanism in TAT current, BTI, and RTN.**

Keywords—HKMG; nMOSFETs; 3D; kinetic Monte-Carlo; multiple traps; coupling; trap generation/recombination; capture time; emission time; threshold voltage shift; trapping; detrapping; PBTI;

I. INTRODUCTION

Bias temperature instability (BTI), random telegraphy noise (RTN), and trap-assisted-tunneling (TAT) induced gate leakage current are major sources of reliability and variability concerns in nano-scaled high-K metal gate (HKMG) MOSFET [1,2]. They are mainly induced by defects trapping/detrapping [3,4]. Single trap analysis is relatively easy to achieve and understand, while multiple trap performance is complex due to the coupling behavior of traps. Moreover, because of the instability of HKMG process and material characteristics, different traps have different response to stress and temperature [5]. In addition, stress inducing new traps in high-K stack has been proved [3,6]. Regarding trapping/detrapping as the result of charging and discharging of oxygen vacancies in HfO_2 is generally accepted [7,8]. Due to the complicated physical phenomenon, it is difficult to extract more detailed information only from measurements. Hence, comprehensive simulation of the traps system is quite necessary to further understand the behavior of multiple traps.

In this paper, a 3D KMC simulator is developed with consideration of coupling characteristics of multiple traps in HKMG nMOSFET. Simulated capture and emission time constants are compared with measurements. Transient characteristics of threshold voltage shift and traps interaction are investigated.

II. SIMULATION METHOD

Fig. 1 shows the schematic of multi-physical models. Capture and emission time constant τ_c and τ_e are obtained by multi-phonon model [9, 10]. Fig. 2 shows the simulation framework, in which probabilities of five processes are described by equation (1)-(10). It presents that trap generation/recombination, trapping/ detrapping to/from channel, metal gate, and the interaction of traps are fully-coupled.

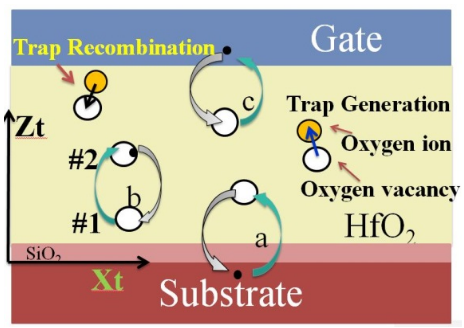

Fig. 1. Schematic of multi-physical models (a: trapping/detrapping from/to channel, b: trapping/detrapping from/to other traps, c: trapping/detrapping from/to channel).

Probabilities of trapping/detrapping are described by following equations:

a: Probability of trapping from Sub （k_c） and detrapping to sub （k_e).

$$k_c = \delta_{nc} v_n \, n \, exp(\beta \varepsilon_{12}) \tag{1}$$

$$k_e = \delta_{ne} v_n N_c \, exp(\beta \varepsilon_{21}) \tag{2}$$

b: Probability of trap i detrapping to trap j （k_{ij}） and trapping from trap j （k_{ji}).

$$k_{ij} = T_{ij} f_c \, exp(\beta \varepsilon_{ij}) \tag{3}$$

$$k_{ji} = T_{ji} f_e \, exp(\beta \varepsilon_{ji}) \tag{4}$$

c: Probability of trapping from gate （k_{cm}） and detrapping to gate （k_{em}).

$$k_{cm} = \delta_{nc} v_n \, n \, exp(\beta \varepsilon'_{12}) \, exp(\alpha x) \tag{5}$$

$$k_{em} = \delta_{ne} v_n N_c \, exp(\beta \varepsilon'_{21}) \, exp(\alpha x) \tag{6}$$

$$\varepsilon_{12} = uc - \lambda (F/F_0)^{\rho} \tag{7}$$

$$\varepsilon_{21} = ue + \lambda (F/F_0)^{\rho} \tag{8}$$

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v_n is thermal velocity ($v_n = \sqrt{8k_BT/\pi m_n}$), m_n is tunneling mass, δ_{nc}, δ_{ne} ($\delta_{nc,e=}\delta_0 T_n$) are capture cross section times. T is temperature. f_c, and f_e are the attempt frequencies. β=–$1/k_BT$. k_BT is the thermal energy; λ and ρ are the enhancement factors of the electric field F, uc and ue are active energies. T_{ij}, T_{ji}, and T_n are the tunneling probabilities, n is the electron density. ε'_{12}, ε'_{21}, ε_{ij} and ε_{ji} are active energies calculated according to nonradiative multiphonon transition models [9].

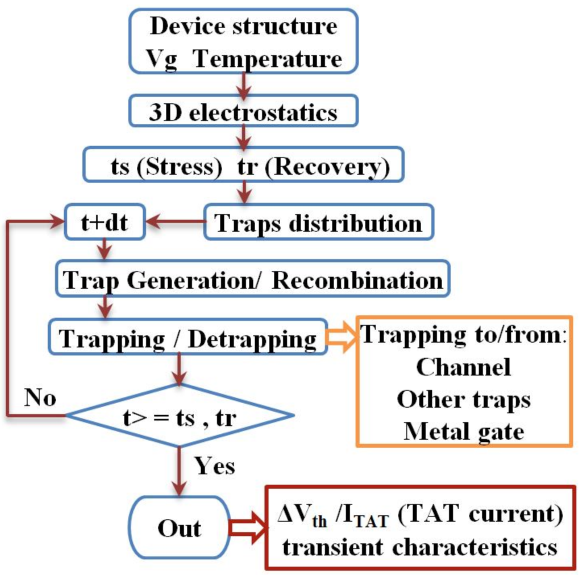

Fig. 2. 3D KMC simulation flowchart.

TABLE I. PARAMETERS IN SIMULATION

Para.	Values	Para.	Values
f_g	5×10^{11} Hz	u_{c0}	0.75 eV
f_r	2×10^{12} Hz	u_{e0}	0.45 eV
$f_{c,e}$	2×10^{13} Hz	σ_c	0.16 eV
λ	0.2eV	σ_e	0.1 eV
F_0	10^2V/cm	ρ	1.5
γ	0.5 nm	α	10^7/cm
m_n	0.18	σ_{Ea} , σ_{Er}	0.2
ε_{HfO2}	22	δ_0	1×10^{-14}cm^2
E_{a0}	1.9eV	u_c, u_e	N($u_{c0,e0}$, $\sigma_{c,e}$)
E_{r0}	1.2eV	E_a , E_r	N($E_{a0,r0}$, $\sigma_{Ea,Er}$)

N(u_0 , σ) is Gaussian distribution. u_0 is mean value. σ is mean-square deviation.

Trap generation probability is given by equation (9) [7], where E_a is the active energy modulated by electrical field . Furthermore, the new instable traps are likely recombination. Probability of trap recombination is determined by active energy E_r and temperature, as shown in equation (10) [11].

e: Probability of trap generation

$$P_g = f_g \exp(\beta(E_a - \gamma F)) \quad (9)$$

f: Probability of trap recombination

$$P_r = f_r \exp(\beta E_r) \quad (10)$$

f_g, f_r are the attempt frequencies and γ is the enhancement factor of the electric field F. Threshold voltage shift ΔV_{th} at time $t+dt$ is obtained by considering the spatial contribution of occupied traps, including pre-existing and new ones. The occupation states of traps are caused by trapping/detrapping from/to substrate/gate/other traps during t to $t+dt$.

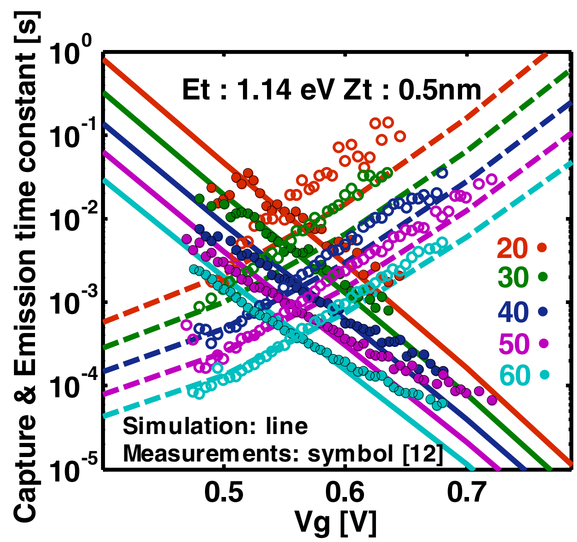

Fig. 3. Single trap τ_c (solid symbol) and τ_e (opened symbol) dependence on gate voltage V_g and temperature

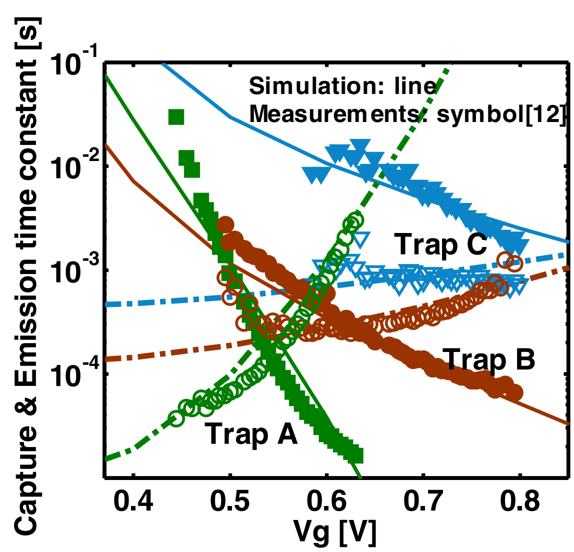

Fig. 4. Three traps τ_c (solid symbol) and τ_e (opened symbol) dependence on gate voltage V_g (Trap A: Et: 0.904eV Zt: 0.25nm; Trap B Et: 1.185eV Zt: 0.5nm; Trap C Et: 1.156eV Zt: 0.75nm).

Fig. 3 shows the simulated capture and emission time constants (τ_c and τ_e) under different temperature, the measurement results in [12] are also plotted, in which τ_e decreases with gate voltage V_g while τ_c increases, indicating that the increase in temperature accelerates trapping/detrapping process. It can be seen that well agreement between the simulation results and the measurement data.

Fig. 4 shows the τ_c and τ_e of three independent traps as functions of V_g, which is in good agreement with experimental data [12]. Simulation results in Fig. 4 indicate differences in location and energy level Et between trap A, B and C. The parameters used in the simulator are listed in Table I.

III. Results and Discussion

In order to investigate the coupling of multiple traps, a 5nm HfO_2 stack with two traps is simulated, as shown in Fig. 1. Fig. 5 shows the ratio of ΔV_{th} to maximum ΔV_{th} in a two-trap system. It can be observed in Fig. 5 that charge exchange between the traps can cause fluctuations in transient waveform of threshold voltage shift. Fig. 6 shows the ΔV_{th} transient characteristics under different capture and emission activation energy (uc and ue) of two traps. It can be seen that τ_c increases with larger activation energy of the capture event and τ_e increases with larger activation energy of emission event. The states of trap #1, #2 are impacted by capture/emission charge from/to channel and each other, simultaneously.

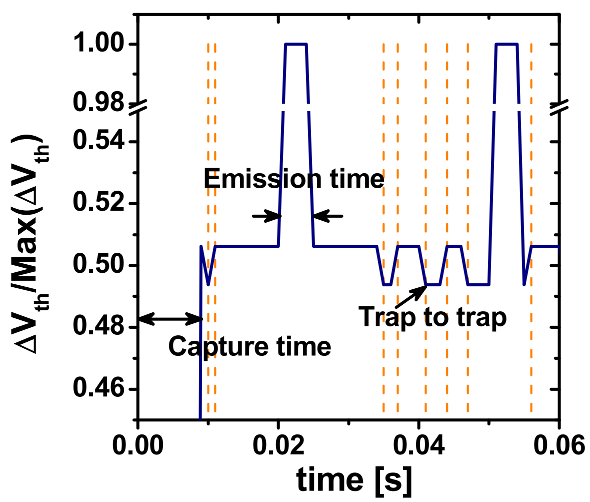

Fig. 5. Trap-to-trap tunneling occur at shallow vertical line

Fig. 7 shows the dependence of trap-to-trap time constant τ_{tt} on the emission (*ue*) and capture (*uc*) active energy. It can be seen that trap-to-trap time constant τ_{tt} (#1 detrapping to #2 or #2 detrapping to #1) increases with larger activation energy of τ_c and τ_e. The time constant of #2 detrapping to #1 is larger than the time constant of #1 detrapping to #2. However, statistical τ_{tt} (average time of exchanging charge) extracted from ΔV_{th} transient characteristics in Fig. 6 decreases at first and then increases from *ue*=0.74eV and *uc*=0.43eV respectively. It indicates that when ue is large enough, the charged traps cannot capture other electrons, while when ue is too small, small charge occupancy rate cannot enable the trap-to-trap tunneling. Similarly, smaller uc results in charged traps while larger uc is related to lower probability of trapping event. It reveals that multiple trap coupling is a compound process with trapping/detrapping from/to gate/channel rather than simple independent event.

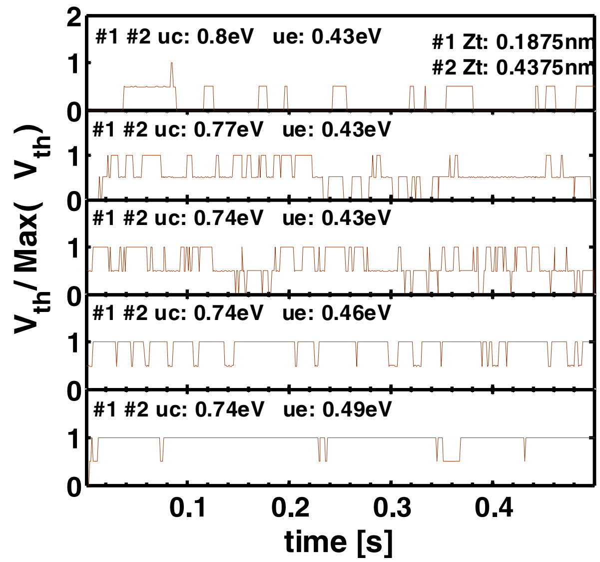

Fig. 6. ΔV_{th} transient characteristic with different uc, ue (V_g=0.6V T=300k, include 2 coupling traps)

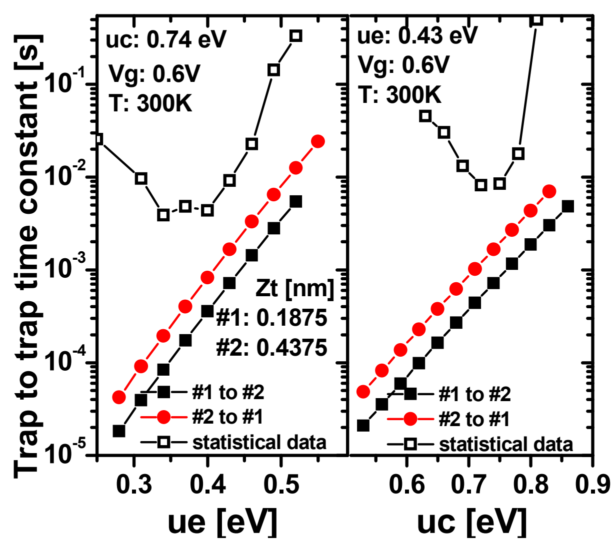

Fig. 7. τ_{tt} dependence on emission (*ue*) and capture *(uc*) active energy

Fig. 8 shows the dependence of trap-to-trap time constant τ_{tt} on distance along Z_t. It can be seen that τ_{tt} increases exponentially with growing distance along oxide thickness Z_t and the tunneling probability increases with larger ΔZ_t (the distance between trap #1 and #2). τ_{tt} of trap #1 to #2 increases more slowly with ΔZ_t than τ_{tt} of trap #2 to #1, while τ_{tt} of trap #2 to #1 have same rate of increase as statistical results.

Fig.9 shows the PBTI phenomenon of nMOSFET induced by the charging events of five traps located at fixed position with Gaussian energy distribution. It indicates that traps with different activation energy result in a obvious difference in threshold voltage shifts. Trapping/Detrapping from/to other traps provide more possibilities of threshold voltage shifts and increase the complexity of analysis.

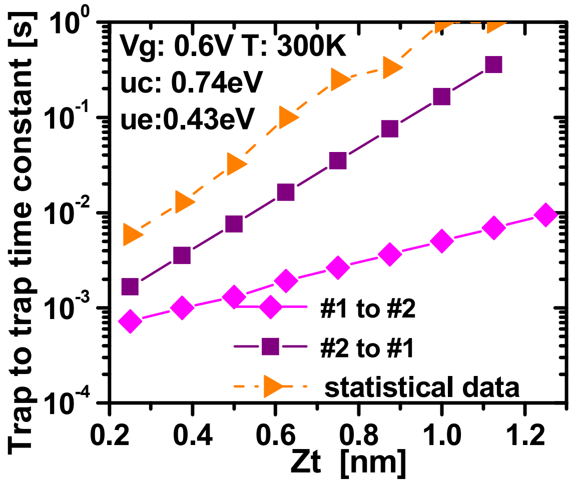

Fig. 8. Trap-to-trap time constant τ_{tt} dependence on distance along *Zt*.

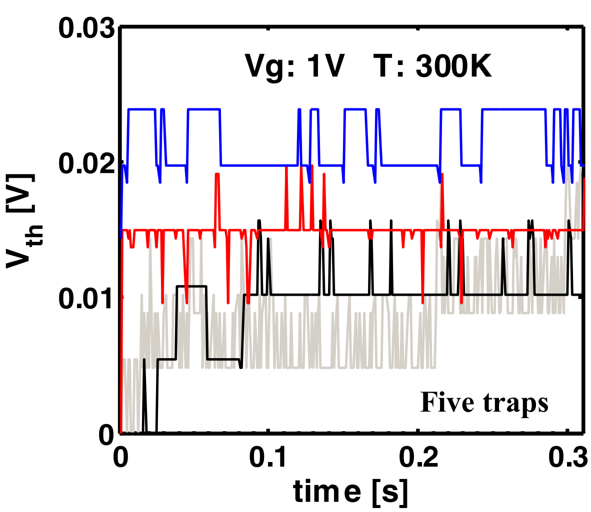

Fig. 9. PBTI induced by trapping (Different colors are related different Gaussian energy distributions. σc=0.16 eV σe=0.1 eV).

IV. SUMMARY

We have modeled the coupling effects of multiple traps and developed a 3D KMC simulator to investigate the multiple traps interaction behaviors. The results indicate that the interaction of multiple traps is much more complex than single trap, which aggravates reliability and variability analysis, induces new mechanism in TAT current, BTI, and RTN. Traps coupling can induce distraction of time constant extraction in measurement especially in material with high trap density.

ACKNOWLEDGMENT

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