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# Characterization and modeling of trap number and creation time distributions under negative-bias-temperature stress

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Individual trapped charge creations and a trap number in p-type metal-oxide-semiconductor field effect transistors (pMOSFETs) under negative bias temperature instability (NBTI) stress are investigated. We find that the characteristic times of a trapped charge creation scatter over several decades of time in small area pMOSFETs, which is attributed to an activation energy distribution in the reaction-diffusion (RD) model of NBTI. We develop a statistical model by combining the RD model with an extracted activation energy distribution to calculate a threshold voltage shift distribution at different NBTI stress times. Our model agrees with measured results very well.

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Negative bias temperature instability has been recognized as a major concern in scaled high-permittivity (high-k) gate dielectric p-type metal-oxide-semiconductor field effect transistors (pMOSFETs) because of its significant impact on circuit performance and reliability.<sup>1-5</sup> As MOSFET dimensions shrink, large variation in negative bias temperature instability (NBTI) induced threshold voltage shifts ( $\Delta V_t$ ) is observed from a device to a device. In device NBTI qualification, since it is the tail part of a  $\Delta V_t$  distribution to determine a qualification pass/failure, an accurate model of an overall  $\Delta V_t$  distribution and its stress time evolutions is urgently needed in an NBTI qualification method. While the mean of an NBTI  $\Delta V_t$  distribution can be well predicted by the reaction-diffusion (RD) model, the RD model alone is insufficient to describe an entire  $\Delta V_t$  distribution. A total  $V_t$  shift in an NBTI stressed device can be expressed as the sum of each individual trapped charge induced  $\Delta v_t$ , i.e.,  $\Delta V_t = \sum_{i=1}^N \Delta v_{t,i}$ , where  $N$  is a total number of stress created trapped charges in a device and  $\Delta v_t$  denotes a single trapped charge caused  $V_t$  shift. Two factors are found to affect a  $\Delta V_t$  distribution. One is the dispersion of  $\Delta v_t$  and the other is fluctuations in number of traps  $N$  in stressed devices. The origin and the distribution of  $\Delta v_t$  have been investigated thoroughly.<sup>3,4</sup> Previous characterization and 3D atomistic simulation show that the  $\Delta v_t$  exhibits an exponential distribution approximately,  $f(|\Delta v_t|) = \exp(-|\Delta v_t|/\sigma)/\sigma$ , due to a random substrate dopant induced current-path percolation effect. To derive a  $\Delta V_t$  distribution, we still need a distribution model for a trapped charge number  $N$ . In literature, a Poisson distribution was usually assumed for  $N$ .<sup>4,5</sup> The Poisson model is based on a notion that individual trapped charge creations during NBTI stress are independent. In other words, each new trap creation in a device has the same probability regardless of how many traps have been created. Nevertheless, the RD model and measurement result show that NBTI trap growth rate obeys a power-law dependence on stress time, i.e.,  $t^{1/n}$  ( $n \sim 6$ ),<sup>6</sup> implying that a new trap creation rate decreases with an increasing trapped charge num-

ber. Therefore, the use of a Poisson model is contradictory to the RD model and may exaggerate  $N$  and a  $\Delta V_t$  distribution tail. In this work, we intend to develop a physics-based distribution model for  $N$  with an extracted activation energy distribution.

We characterize NBTI trapped charge creation in high-k (HfO<sub>2</sub>) gate dielectric and metal gate pMOSFETs. The devices have a drawn gate length of 30 nm, a gate width of 80 nm and an effective oxide thickness of 0.8 nm. Our characterization consists of two alternating phases. In NBTI stress phase,  $V_{gs} = -1.8$  V and  $V_d = 0$  V. In measurement phase, the drain voltage is  $-0.05$  V and the gate voltage is adjusted to have a drain current of  $\sim 500$  nA in a fresh device. Drain current variations in NBTI stress are traced with a switch delay time less than 1  $\mu$ s using Agilent B1500. A corresponding  $\Delta V_t$  trace is obtained from a measured  $\Delta I_d$  divided by a transconductance. Fig. 1 shows representative  $V_t$  traces in two devices during NBTI stress. Each sudden  $V_t$  change ( $\Delta v_t$ ) in the traces is due to a single trapped hole creation. We collect about 900  $\Delta v_t$  in  $\sim 130$  devices. The extracted  $\sigma$  is about 3.3 mV. In addition, individual trapped charge creation times are clearly defined in the figure. We collect the first three charge creation times in about 130 devices. The trap creation characteristic times scatter over several decades of time.

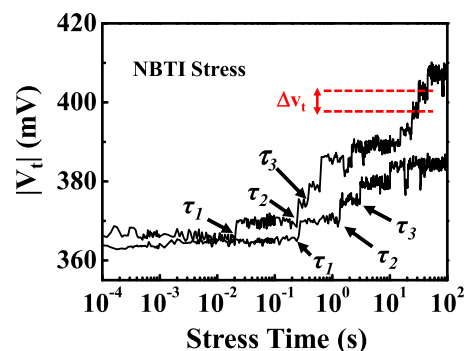


FIG. 1.  $V_t$  traces during NBTI stress in two high-k (HfO<sub>2</sub>) gate dielectric and metal gate pMOSFETs.  $\tau_1$ ,  $\tau_2$ , and  $\tau_3$  are the 1st, the 2nd, and the 3rd trapped hole creation times.  $\Delta v_t$  is a single trapped charge induced threshold voltage shift.

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Their probability density functions (PDF) are shown in Fig. 2. The wide spread of the characteristic times is attributed to an activation energy distribution in the RD model due to local chemistry because other processes or variables in the RD model are unlikely to cause such wide distributions. In the following, we will extract an activation energy distribution from the measured trap characteristic time distributions.

According to the RD model, an NBTI trap creation rate is formulated as

$$N = A \frac{1}{n} \exp\left[\frac{-E_a}{k_B T}\right], \quad n \sim 6, \quad (1)$$

where

$$A \equiv WLD_0^{1/6} \left[ \frac{K_{F0}[SiH][h^+]}{pK_{R0}} \right]^{2/3}. \quad (2)$$

$W$  is a gate width,  $L$  is a gate length, and other variables have their usual definitions as in Ref. 6. Three activation energies ( $E_F$ ,  $E_R$ ,  $E_{diffusion}$ ) associated with  $K_F$ ,  $K_R$ , and  $D$  in the RD model are lumped together and effective activation energy ( $E_a$ ) in Eq. (1) is defined as<sup>6</sup>

$$E_a = \frac{1}{6}E_{diffusion} + \frac{2}{3}(E_F - E_R). \quad (3)$$

By re-arranging the terms in Eq. (1), the relationship between effective activation energy and the  $i$ th trapped charge creation time ( $\tau_i$ ) is shown below

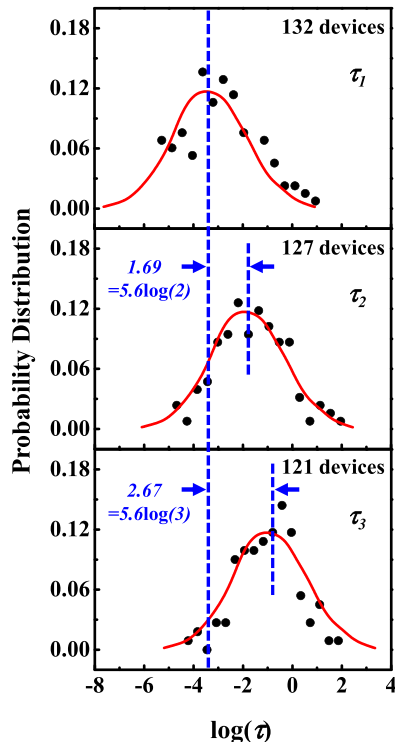


FIG. 2. The probability distribution of a trapped charge (hole) creation time in NBTI stress.  $\tau_1$ ,  $\tau_2$ , and  $\tau_3$  are the 1st, the 2nd, and the 3rd trapped hole creation times, respectively, in a device. The three  $\log(\tau)$  distributions have a similar shape but are shifted by an amount  $n\log(i)$ .

$$E_a = \frac{2.3k_B T}{n} [n\log(A) + \log(\tau_i) - n\log(i)]. \quad (4)$$

Thus, we can extract a relative activation energy distribution from the measured  $\log(\tau_i)$  by subtracting  $n\log(i)$  from it. According to our measurement data,  $n$  is about 5.6 in the initial stress stage, which is slightly different from  $n=6$  in the RD model. The  $\log(\tau_i) - n\log(i)$  and corresponding activation energy distributions from the  $\tau_1$ ,  $\tau_2$ , and  $\tau_3$ , respectively, are shown in Fig. 3. The top X-axis in Fig. 3 denotes extracted  $E_a$  according to Eq. (4). The pre-factor  $A$  is chosen such that the mean of the  $E_a$  is consistent with a published result in Ref. 7. A reasonably good match of the activation energy distributions from the  $\tau_1$ ,  $\tau_2$ , and  $\tau_3$  is obtained. The solid line in Fig. 3 represents a Gaussian-distribution fit. The mean of the Gaussian distribution is  $\mu(E_a) = 0.12$  eV and the standard deviation is  $\sigma(E_a) = 0.015$  eV.

A statistical model based on a Monte Carlo (MC) approach is developed to calculate  $N$  and  $\Delta V_t$  distributions. In our MC simulation, a sequence number ( $i$ ) is assigned to each precursor in a device. The number of precursors is set equal to  $M=24$  in a  $80\text{ nm} \times 30\text{ nm}$  device, which corresponds to a precursor density of  $10^{12}\text{ cm}^{-2}$ .<sup>8</sup> Each trapped charge creation time ( $\tau_i$ ) is then calculated according to Eq. (4) by randomly selecting an  $E_a$  from the Gaussian distribution. In this approach, we can reproduce the same  $\tau_i$  distributions as in Fig. 2. For a stress time  $t$ ,  $N$  is computed by counting all the precursors with  $\tau_i$  ( $i=1,2,\dots,24$ ) less than  $t$ . For each counted precursor, a  $\Delta V_t$  is randomly selected based on the distribution  $f(|\Delta V_t|) = \exp(-|\Delta V_t|/\sigma)/\sigma$  with  $\sigma = 3.3$  mV. In total,  $5 \times 10^5$  devices are simulated in the MC simulation. The simulated and measured  $\Delta V_t$  distributions are shown in Fig. 4 at a stress time of  $t = 1$  s and 100 s. Good agreement between the Monte Carlo simulation and measurement is obtained. Finally, we compare this model with the Poisson distribution model at a stress time of 100 s. To highlight the difference between the two models, only the tail part of a complementary cumulative distribution function (1-CDF) of the  $\Delta V_t$  is shown in Fig. 5. A  $\Delta V_t$  distribution based on the Poisson model is also shown in Fig. 5 for comparison. In addition, trap number distributions from the two models are plotted in the inset. The Poisson model apparently yields a broader distribution in  $N$  and thus a larger  $\Delta V_t$ .

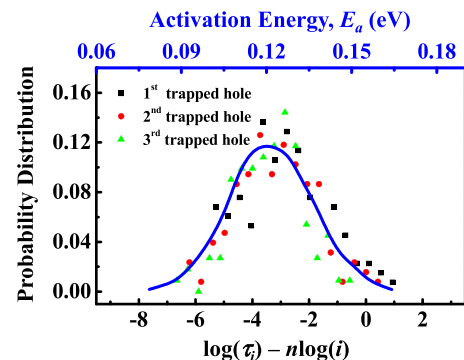


FIG. 3. The probability distributions of  $\log(\tau_i) - n\log(i)$  (bottom X-axis) and corresponding activation energy ( $E_a$ ) (top X-axis). The pre-factor  $A$  in Eq. (4) is chosen such that the mean of the  $E_a$  is about 0.12 eV. The solid line represents a Gaussian-distribution fit.

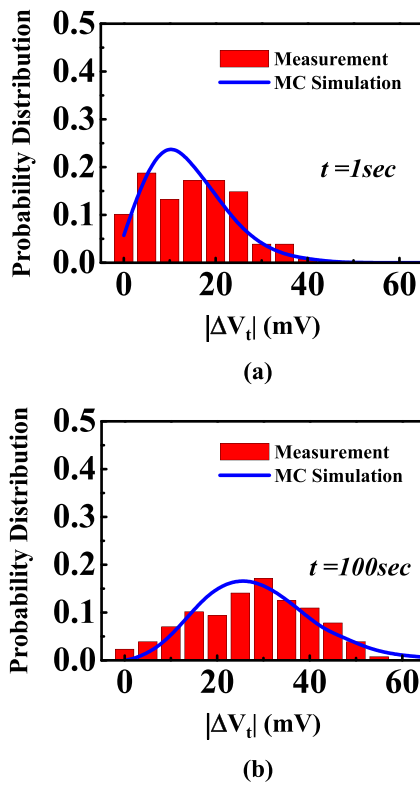


FIG. 4. NBTI induced  $\Delta V_t$  distributions from measurement and from a Monte Carlo simulation. The stress time is 1 s (a) and 100 s (b), respectively.

tail, as explained earlier. The difference between the two models increases as more trapped charges are created.

In summary, we characterize NBTI trap creation in a large number of high-k dielectric pMOSFETs. An activation energy distribution in the RD model is extracted. We propose a statistical model for a trap number distribution. Our model can be used to predict an NBTI  $\Delta V_t$  distribution and its stress time evolutions.

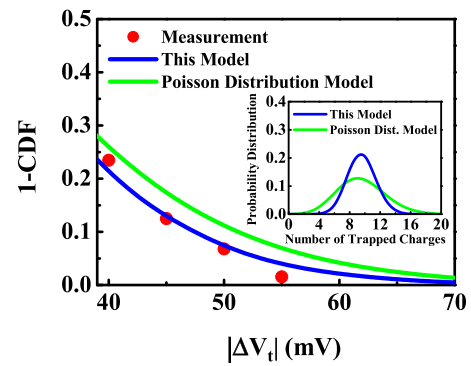


FIG. 5. Comparison of NBTI induced  $\Delta V_t$  distributions (1-CDF) calculated from this model and from the Poisson model. The dots are measurement data points. Only the tail part of the 1-CDF is drawn to highlight the difference between these two models. The inset shows trapped charge number distributions from the two models. The stress time is 100 s.

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