Simulation of Reliability on Nanoscale Devices

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Abstract—We study the trapping kinetics of oxide traps and the subsequent degradation in p-channel MOSFET under bias temperature stress and in presence of random discrete dopants. Using our simulator Minimos-NT we self-consistently undertake time-dependent simulations of defect creation employing our multistate non-radiative multi phonon model. We find that random discrete dopants shift and broaden the distribution of the trapping time constants resulting in lower ∆Vth than one would obtain without random discrete dopants. Additionally, the influence of self-consistency on the trapping kinetics is investigated.

I. INTRODUCTION

Recent studies have demonstrated that in modern decanometer devices the variability due to random discrete dopants (RDD) and oxide defects has become critical in the context of reliability [1]–[4]. For instance, discrete charges in the oxide or at the interface lead to the occurrence of potentially huge ∆Vth shifts due to the non-uniform current flow in the channel (Fig. 1). Previous studies have considered either fixed positive/negative charges or described charge capture into a fixed number of defects by standard SRH trapping kinetics [5]. However, the actual number of available defects is time-dependent and their activation process itself might be sensitive to the microscopic configuration of the channel. Also, recent studies on charge trapping during random telegraph noise (RTN) and the recoverable component of the bias temperature instability (BTI) have shown that the phenomenon is more complicated than anticipated in the SRH model, requiring metastable defect states and non-radiative multi phonon (NMP) transitions between the states [6], [7].

II. METHOD

For our self-consistent time-dependent simulations of oxide defect creation, as well as charging and discharging of created defects contributing to the recoverable component of BTI, we employ our recently proposed multistate NMP model (Fig. 2). Random discrete dopants are considered using the method from [8] with a density gradient (DG) quantum correction model [9]. The maximum number of traps in the gate oxide is determined using Poisson statistics and the direct method [10] for calculating random numbers according to a given Gaussian probability density function (pdf). The spatial positions of the traps as well as the adiabatic potentials describing the kinetics are then randomly chosen using the described method. In order to have realistic trap-parameters for the NMP model, parameters close to those used in a previous study [6] (defect #1) have been employed as mean values for the trap-distribution (cf. Tab. I).

TABLE I: The parameters of the multistate NMP model (Fig. 2) used in this study. The trap levels E1 and E2 have the largest standard deviations. This will result in a few traps being more likely in state 1’ than in state 1 before stress.

The small standard deviations have been arbitrarily chosen such, that after short stress times the onset of saturation of the degradation can be readily observed. The device under test is a p-channel MOSFET with a channel length of 60 nm,
Fig. 3: The oxide trap model from [6]. The sketch shows a finite state diagram for a single defect, in which state 1 is the stable and electrically neutral precursor state. Upon hole capture (red arrow from state 1 to state 2) the defect becomes positively charged but remains meta-stable. A defect in state 1′, upon the capture of an electron, undergoes a transition back to the neutral and stable precursor state 1. The charge carrier exchange processes with the substrate are modeled using NMP theory [11], [12]. Alternatively, a defect in state 2 can undergo the slow process of structural relaxation, become stable and stay positively charged (state 2), which was for example used to explain DCIV experiments [13]. In state 2 the defect can either go back into state 2′ or can capture an electron thus becoming electrically neutral and return to state 1′. In state 1′ the defect is neutral and can either by structural relaxation undergo a transition into the stable precursor state 1 or can capture a hole and thus change into the stable positively charged state 2.

Fig. 4: Same as in Fig. 3, but with DD and no RDD. The average number charged traps is 10% larger at the end of stress (at 100 seconds) compared to Fig. 3.

Fig. 5: The time evolution of the trapped charges (ΔVth) simulated utilizing a DD approach for 200 microscopically different devices. After bias temperature stress has been applied the first traps with a small capture time constant are filled. At the end of the experiment (100 seconds) the degradation begins to saturate.

Fig. 6: The time evolution of the average trapped charge for a single device considering RDD. There is a time-delay of three orders of magnitude between the onset of stress and the first trapped charges.

an effective oxide thickness of 2 nm with an average of twenty seven possible traps uniformly distributed in the oxide, corresponding to a density of $1.5 \times 10^{18}$ cm$^{-3}$.

III. RESULTS

First, BTI stress experiments are simulated for two hundred microscopically different devices with and without RDD using our NMP model. Before applying a stress field of approximately 8 MV/cm, the device is assumed to be in equilibrium at a stress temperature of 125 °C with all contacts grounded and no charged oxide traps. The average degradation in terms of trapped charges is approximately 10% lower when RDD are considered (Fig. 3 and Fig. 4). When RDD are considered, the onset of degradation is delayed in comparison to the case where RDD are not considered (Fig. 3). This is dominantly due to the strong sensitivity of the capture and emission time constants of the various defects to the random surface potential. Thus it is necessary to consider the influence of random dopants in sub-100 nm devices, when investigating bias temperature instability. This becomes more evident if two simulations with and without RDD (Fig. 5 and Fig. 6) of the ensemble are compared and is also a direct consequence of
the change in capture time constants of the various oxide traps (cf. Tab. II).

<table>
<thead>
<tr>
<th>Parameter</th>
<th>( \mu [s] )</th>
<th>( \mu_{\text{RDD}} [s] )</th>
<th>( \sigma [s] )</th>
<th>( \sigma_{\text{RDD}} [s] )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \tau_c )</td>
<td>29.0</td>
<td>( 3.59 \times 10^4 )</td>
<td>8.69 \times 10^3</td>
<td>1.37 \times 10^7</td>
</tr>
</tbody>
</table>

**TABLE II:** The mean values of the capture time constant \( \tau_c \) and the respective standard deviations without and with RDD.

Upon inspecting the capture and emission time constants for the whole ensembles without RDD (Fig. 7) and with (Fig. 8) the aforementioned shift in capture time constants \( \tau_c \) towards higher capture times is visible. Additionally the distribution of capture time constants is broader when considering RDD compared to the simulations where RDD have been neglected. This can be explained with the high sensitivity on the potential of the NMP charge capture process for a single defect between state 1 and 2’ (cf. Fig. 2) [7]. Another notable fact is that due to the random potential fluctuations caused by the random discrete dopants, the device degradation at the end of stress is less severe compared to the case where RDD are not considered (Fig. 8). This is a direct consequence of the NMP charge capture process and would not be observable for SRH.

In order to assess the significance of the influence of the observed effects, a CMOS inverter with a p-channel MOS under BTI stress is simulated in mixed device/circuit mode (cf. Fig. 9). It can be clearly seen that due to the wide distribution of time constants treating traps as fixed charges gives a more pessimistic device behavior compared to the device behavior under more realistic dynamic trapping conditions. In particular, many defects are too slow to follow the rapid changes of the surface potential. In contrast, the time constants predicted by a SRH model are very small and do not capture this effect [7].

**IV. CAPTURE AND EMISSION TIME CONSTANTS**

One particularly important consequence of the self-consistent solution scheme employed here is that the capture and emission times can change during the simulated stress, in particular, \( \tau_c \) may shift to larger values. Two cases have to be contrasted here: In case one, \( \tau_c \) shifts because a neighboring defect becomes charged. In case two, \( \tau_c \) can change due to an artificial self-interaction with its partial charge stored in the defect. As a consequence, the charging characteristics of such defects may no longer follow the familiar first-order form \( \Delta V_{\text{th}} = A (1 - \exp (-t/\tau)) \). A statistical analysis of the number of defects deviating from the first-order form is given in Fig. 11. It is important to note that in all self-consistent simulations the time capture \( \tau_c \) and emission constants \( \tau_e \) of the vast majority of defects did not, within numerical reasonable bounds, change. The observed symptom of trap-self-interaction is a change in time constants which occur smoothly over stress time while the probability of the trap being occupied by a charge carrier increases. This is due to the high sensitivity of \( \tau_c \), calculated according to NMP theory, on the potential and due to our approach in which we incorporate self-consistency in a continuous manner by introducing the expected trap charge of the stochastic process. A discrete trap can either be charged by an electron or hole or empty. Thus a self interacting trap will exhibit a strong deviation from the experimentally observed first order kinetics (cf. Fig. 10). Such self interactions of traps must be avoided during simulation or assessed, using a proper techniques, after simulation. One way to avoid self-interaction is to use a Monte Carlo approach for which self interaction can be intrinsically avoided. A way to check an ensemble of self-consistent simulations employing the potential sensitive NMP model for artifacts after simulation is to plot the cumulative distribution of the time it takes each trap to change its occupancy from 10% of its initial value to 90% of its final value (cf. Fig. 11). When using SRH theory, where \( \tau_c \) linearly depends on the surface potential, instead of NMP theory one will find that the influence of self-interaction is minimal.

**V. CONCLUSION**

We have studied the impact of RDD on the dynamics of trap creation in a self-consistent manner. Our results demonstrate that RDD can lead to a significant reduction in the total
overestimates the degradation. The input/output curve of CMOS inverter, where the p-channel MOS is subjected to BTI stress at $V_{gs} = -1.0\, V$. It can be seen that, repeating the simulation in 3D with RDD and fixed oxide charges (traps) clearly overestimates the degradation.

The probability of a single self interacting trap to be occupied by a hole over stress time. The red curve is the occupancy for a self-consistent charging process. As a reference the blue curve shows the expected charging behaviour of the trap.

Fig. 11: The cumulative distribution function for the time it takes each trap to change its occupancy from 10% of its initial value to 90% of its final value on a log-scale (cf. inset) for the whole ensemble of discrete traps in all 200 simulations. Since significantly more than 90% of all 2600 traps exhibit self interaction, when treating the occupancy in a continuous manner.

$\Delta V_{th}$ after degradation. This reduction is due to two effects, namely the sensitivity of the capture time constants of the defects to the random surface potential as well as a reduction of the average $\Delta V_{th}$ per defect, which dominates over the increased probability of the occurrence of giant $\Delta V_{th}$ steps. We have also shown that treating traps as fixed charges results in a pessimistic estimate for circuit degradation, since only a fraction of the created defects is able to follow rapid changes in the surface potential. Thus in order to correctly account for device degradation ($\Delta V_{th}$) in BTI experiments and the simulations of whole circuits, traps and their kinetics must be included in a self-consistent manner. Furthermore we investigated the sensitivity of the capture and emission times on random dopant fluctuations and the possibility of self interaction, when treating the occupancy in a continuous manner.

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REFERENCES


