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 ΔV_{th} 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 deca-nanometer 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 ΔV_{th} 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 meta stable 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).

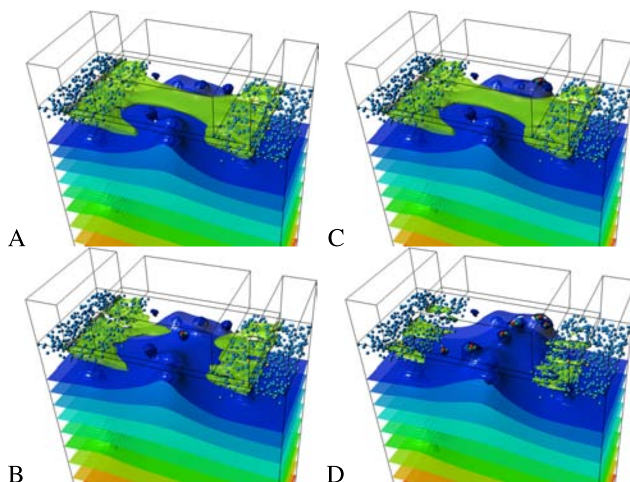

Fig. 1: The percolation path in a selected microscopic p-channel MOS due to random discrete dopants and equipotential surfaces. In subfigure A there are no oxide traps and a single percolation path dominates. Upon the the formation of a fully charged trap right above the dominant percolation path, the device is switched off and the dominant percolation path vanishes (subfigure B) leading to a huge ΔV_{th}. When an oxide trap is being charged next to the percolation path (subfigure C), the trap has a negligibly small influence on the current flow and causes only a small ΔV_{th}. Subfigure D shows the formation of six fully charged traps perpendicular to the current flow. In such a case the device becomes much harder to turn on.

Parameter	Mean Value μ	Standard Deviation σ
E_{t}	0.6 eV	0.1 eV
E'_{t}	0.75 eV	0.1 eV
R	0.5	0.01
S	0.6	0.01
R'	0.8	0.01
S'	0.6	0.01
ϵ_{T2}	0.5 eV	0.05 eV
$\epsilon_{1'1}$	0.8 eV	0.05 eV
$\epsilon_{2'2}$	0.5 eV	0.05 eV

TABLE I: The parameters of the multistate NMP model (Fig. 2) used in this study. The trap levels E_{t} and E'_{t} 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 $60\ \mathrm{nm}$,

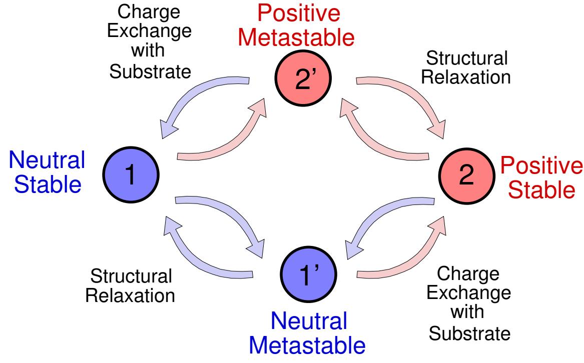

Fig. 2: The oxide trap model from [6]. The sketch shows a finite state diagram for a single defect, in which state 1 is the stable and electrically neutral precursor state. Upon hole capture (red arrow from state 1 to state $2'$) the defect becomes positively charged but remains meta-stable. A defect in state $2'$ can, upon the capture of an electron, undergo 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.

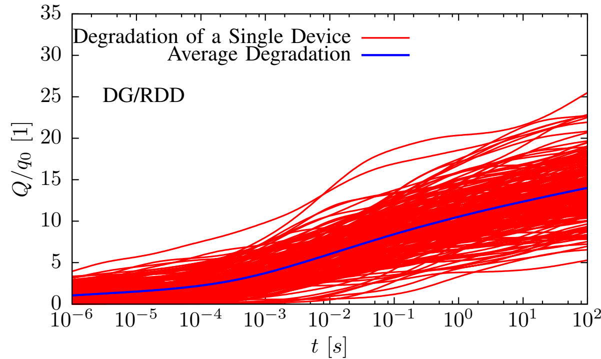

Fig. 3: A simulated BTI stress experiment for 200 microscopically different devices using a NMP model, DG and RDD.

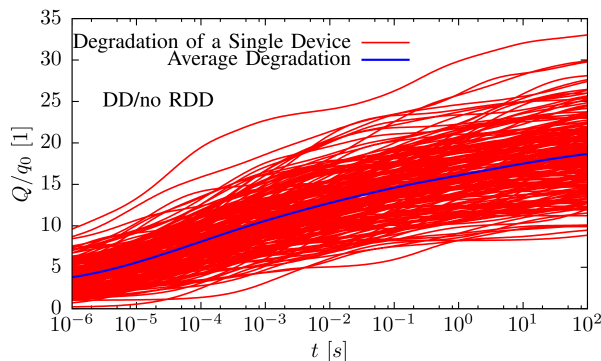

Fig. 4: Same as in Fig. 3, but with DD and no RDD. The average number charged traps is 10% larger at the end of stress (at 100 seconds) compared to Fig. 3.

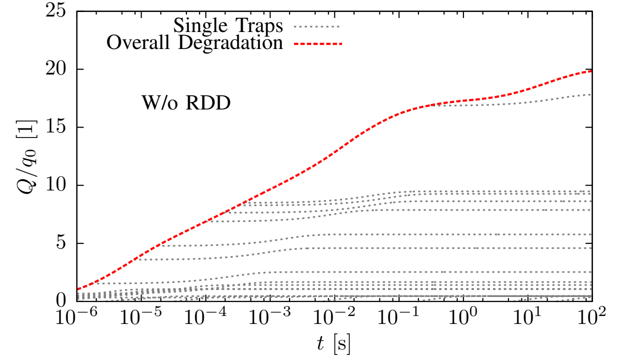

Fig. 5: The time evolution of the trapped charges (ΔV_{th}) simulated utilizing a DD approach for 200 microscopically different devices. After bias temperature stress has been applied the first traps with a small capture time constant are filled. At the end of the experiment (100 seconds) the degradation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

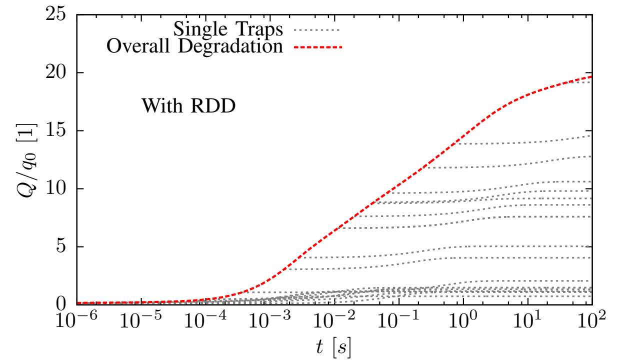

Fig. 6: The time evolution of the average trapped charge for a single device considering RDD. There is a time-delay of three orders of magnitude between the onset of stress and the first trapped charges.

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

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 $8\,\mathrm{MV/cm}$, the device is assumed to be in equilibrium at a stress temperature of $125\ °\mathrm{C}$ 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).

Parameter	μ [s]	μ_{RDD} [s]	σ [s]	σ_{RDD} [s]
τ_{c}	29.0	3.59×10^{3}	8.69×10^{4}	1.37×10^{7}

TABLE II: The mean values of the capture time constant τ_{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 τ_{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, τ_{c} may shift to larger values. Two cases have to be contrasted here: In case one, τ_{c} shifts because a neighboring defect becomes charged. In case two, τ_{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 $\Delta V_{\mathrm{th}} = A\left(1-\exp\left(-t/\tau\right)\right)$. 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 τ_{c} and emission constants τ_{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 the high sensitivity of τ_{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

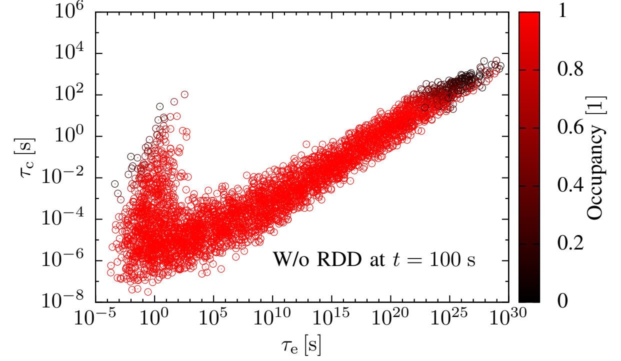

Fig. 7: For each trap in one of the 200 devices with continous doping the occupancy of each trap after 100 seconds of bias temperature stress is shown (color coded). In can be seen that traps with a massively high emission time constant, which correspond to a more permanent degradation, are occupied. In this study the capture time constants have been chosen to be within the stress time in order to demonstrate saturation.

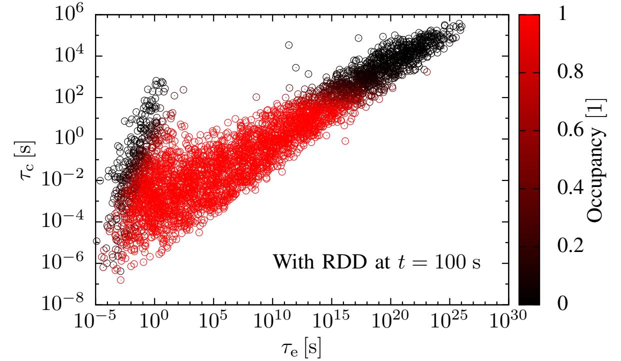

Fig. 8: The same as in Fig. 7 after 100 seconds of bias temperature stress, but considering RDD. Due to the shift in time constants, especially in the capture time constants, caused by the RDD less traps are occupied than when using continous doping (cf. Fig. 7).

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 assesed, 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 τ_{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

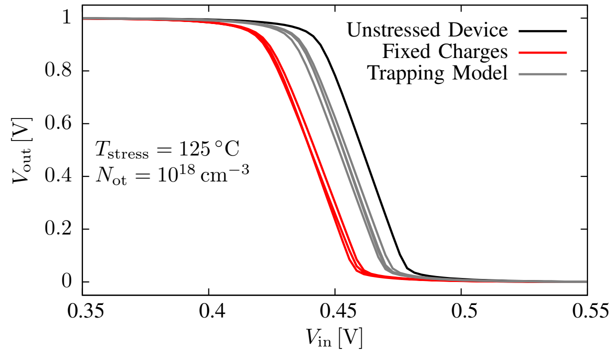

Fig. 9: The input/output curve of CMOS inverter, where the p-channel MOS is subjected to BTI stress at $V_{gs} = -1.0\,\mathrm{V}$. It can be seen that, repeating the simulation in 3D with RDD and fixed oxide charges (traps) clearly overestimates the degradation.

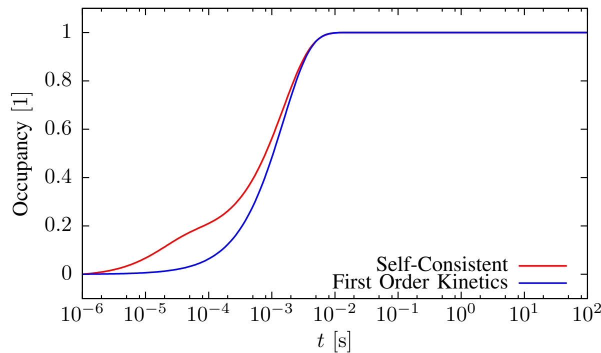

Fig. 10: The probability of a single self interacting trap to be occupied by a hole over stress time. The red curve is the occupancy for a self-consistent solution entering fractional charges leading to a trap self interaction during the charging process. As a reference the blue curve shows the expected charging behaviour of the trap.

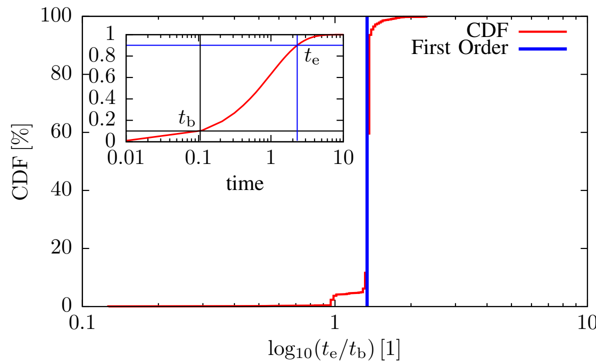

Fig. 11: The cumulative distribution function for the time it takes each trap to change its occupancy from 10% of its initial value to 90% of its final value on a log-scale (cf. inset) for the whole ensemble of discrete traps in all 200 simulations. Since significantly more than 90% of all 2600 traps exhibit the expected first oder behavior the influence of the self interacting traps is negligible.

ΔV_{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 ΔV_{th} per defect, which dominates over the increased probability of the occurrence of giant ΔV_{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 (ΔV_{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.

VI. Acknowledgment

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