

# Evidence That Two Tightly Coupled Mechanisms Are Responsible for Negative Bias Temperature Instability in Oxynitride MOSFETs

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**Abstract**—Negative bias temperature instability (NBTI) is a serious reliability concern for pMOS transistors. Although discovered more than 40 years ago, the phenomenon remains highly controversial in both experimental and theoretical terms. A considerable number of recent publications suggest that NBTI is caused by the following two *independent* mechanisms: 1) generation of defects close to the silicon/silicon dioxide interface and 2) hole trapping in the oxide. We have performed stress and recovery experiments at different temperatures and voltages that, quite surprisingly, reveal that all data can be scaled onto a single universal curve during stress, recovery, and restress. This suggests that in our samples, NBTI is caused by either a single dominant mechanism, which is more complicated than previously anticipated, or that the previously suggested mechanisms, i.e., hole trapping and defect creation, are actually tightly coupled.

**Index Terms**—Dangling bonds,  $E'$  centers, hole trapping, interface states, negative bias temperature instability (NBTI), oxide charges, reaction-diffusion theory.

## I. INTRODUCTION

APPLICATION of a negative bias to the gate of an otherwise grounded pMOS transistor results in the degradation of crucial transistor parameters such as threshold voltage and mobility. Because this degradation is accelerated by temperature and bias, this phenomenon has become known as negative bias temperature instability (NBTI) [1]. The current understanding is that the degradation is caused by the creation of defects at the Si/SiO<sub>2</sub> interface [2] and possibly by holes trapped in the dielectric [3]–[5]. For devices using nitrided oxides, it has been suggested that the defects are predominantly created inside the dielectric [6]. Furthermore, it has been suggested that the processing of the nitrided layer can have a fundamental impact on its reliability [5], with thermal nitridation resulting in a considerably larger susceptibility to NBTI than plasma nitridation. This has been attributed to a larger hole trapping component in thermally nitrided samples.

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Unfortunately, measuring the true degradation caused by NBTI is exceedingly complicated, if not impossible, due to the fast recovery of the degradation setting in at time scales smaller than a microsecond [7] and the strong sensitivity of the recovery to the applied bias voltage, particularly to positive voltages. Altogether, it has been understood that any experimental assessment is imperfect [8]–[10], while the degree of distortion inherent to each technique is still under debate.

While many older studies have related NBTI solely to the creation of interface states [11], [12], the introduction of fast measurement techniques during both stress and relaxation has revealed considerable discrepancies with the predictions given by the classic reaction–diffusion (RD) theory [7], [13]. Consequently, much recent research effort has discussed the impact of additional hole trapping into preexisting traps [4], [5], [14], [15]. These conclusions were reached by studying both the stress and the relaxation phase with some interesting aspects summarized as follows.

- 1) During the initial stress phase, it has been speculated that the filling of preexisting traps results in a temperature-independent contribution, which is given by a logarithmic time dependence [5], [7], [9], [16]. After this initial phase, which has sometimes been assumed to be relatively short ( $<1$  s) [10], it has been suggested that the degradation is dominated by the generation of interface states, either via dispersive bond breaking [13], [17] or via the mechanism postulated by the RD theory [11], [18], [19]. In the latter case, the coexistence of these two mechanisms has been used to explain smaller power-law exponents (slopes) than those theoretically possible according to the RD theory, most notably the celebrated  $n = 1/6$  [10].
- 2) Detailed studies of the recovery phase [4], [15], [20] have revealed that the recovery may be expressed as a superposition of a quickly recoverable and a nearly permanent component. Again, not surprisingly, these two components have been assigned to hole trapping and interface state generation. Interestingly, however, there is no agreement on which physical process is responsible for which component and the permanent component has been assigned to both interface state generation [4] and holes trapped in deep energetic states [15].

Disregarding the aforementioned contradictions for the moment, we summarize two different models. One is based on the

ideas of Haggag *et al.* [17] and Huard *et al.* [4], [13], who model the overall degradation during stress as

$$\Delta V_{th}(t_s) \sim \frac{A_{it}}{1 + (t_s/\tau_{it})^{-\alpha}} + A_h \log \left( 1 + \frac{t_s}{\tau_h} \right) \quad (1)$$

with  $A_{it} = A_{it}(V_{stress}, T)$  and  $A_h = A_h(V_{stress}, T)$  being the temperature- and voltage-dependent prefactors for interface state generation and hole trapping, where the temperature dependence of the latter is commonly assumed to be small [7]. According to the dispersive first-order reaction assumed to be responsible for the creation of interface states, the time constant  $\tau_{it}(V_{stress}, T)$  is also a function of both the temperature and the stress voltage [21]. Furthermore, the exponent  $\alpha$  has been expressed as a linear function of temperature, i.e.,  $\alpha = k_B T / \sigma$ , with  $\sigma$  being the variance of the Gaussian distribution of the binding energies. The time constant for the buildup of charge inside the oxide  $\tau_h$  is also assumed to be only weakly temperature dependent.

Alternatively, models based on the RD theory with superpositioned hole trapping [10] postulate the following time dependence of the degradation:

$$\Delta V_{th}(t_s) \sim A_{it} t_s^n + A_h \log \left( 1 + \frac{t_s}{\tau_h} \right). \quad (2)$$

Although those works do not explicitly specify the functional form of the hole trapping term, we also write it using the same expression as in (1), as this captures the basic idea. Again, the prefactor for interface state generation depends on both temperature and voltage, i.e.,  $A_{it} = A_{it}(V_{stress}, T)$ , while  $n$  is a firm constant (1/6), at least in the basic  $H_2$  model formulation. Such a constant (voltage and temperature independent) exponent  $n$ , although with a smaller value than 1/6 (0.1, ..., 0.14), appears to be in agreement with experimental data [5].

Irrespective of the question whether (1) or (2) is closer to experiment, their functional form suggests the following.

- 1) Both components are of the same order of magnitude; otherwise, one of the processes would be dominant and the other irrelevant.
- 2) The two components should be separable by applying stresses at different voltages and temperatures because the temperature and voltage dependence of such diverse phenomena as interface state generation and hole trapping is likely to be diametrically different. In fact, the hole trapping component is commonly assumed to be temperature independent [5], [7], [10], [13], while activation energies of about 60–100 meV [5], [22], [23] have been given for the creation of interface states. It has also been observed that the creation of interface states follows a non-Arrhenius temperature dependence [13].

Based on these notions, we have performed a number of experiments in order to check whether such a separation based on different voltage and temperature dependences is indeed possible. In contrast to some previous studies, we take care not to base our conclusions on a comparison of inherently different experiments, such as conventional electrical measurements and charge pumping (CP) [13], [15]. Although we believe that CP experiments can provide valuable insight into the bias tempera-

ture instability, we have to keep in mind that CP measurements are extremely invasive due to the application of positive bias. Currently available theories cannot properly account for these bias conditions, particularly for the experimentally observed accelerated recovery [13], [24]. While it is clear that CP scans a different fraction of the bandgap [5], a rigorous link between the CP current and  $\Delta V_{th}$  still needs to be established.

## II. EXPERIMENTAL

In the following, we therefore employ our extended measure/stress/measure technique (eMSM) [24]–[26], which records the change in  $V_{th}$  during subsequent stress and relaxation sequences in order to maximize the characterization data obtainable for a single device in a single measurement sequence.

- 1) During exponentially growing stress intervals, drain-current degradation is recorded, which mimics conventional on-the-fly (OTF) measurements. Since the drain-current is recorded during both the stress and relaxation phases, a constant drain bias of  $-50$  mV is maintained during the whole measurement run. The degradation of the drain-current is then converted to [27]

$$\Delta V_{th}^{OTF} \approx \frac{I_D - I_{D0}}{I_{D0}} (V_G - V_{th0}^{OTF}) \quad (3)$$

which is a quantity often assumed to have similar properties as the threshold voltage shift  $\Delta V_{th}$ .  $I_{D0}$  is the undegraded value of the drain-current at stress level, which is a difficult-to-obtain quantity [9], while  $V_{th0}^{OTF}$  is the threshold voltage of the virgin device. For some time, OTF measurements have been considered as the only proper characterization method for NBTI since the technique does not suffer from artifacts due to recovery. In fact, it is now understood that  $\Delta V_{th}^{OTF}$  is contaminated by mobility variations and the error in  $I_{D0}$  [8]–[10]. Correction schemes for these errors have been suggested [10], [28] but are still open to rigorous justification.

- 2) After each stress interval, in our particular case at 2, 15, 60, 230, 740, 2000, and 6000 s, the gate voltage is switched from the stress voltage to the (temperature dependent) measurement voltage close to the initial threshold voltage  $V_{th0}$ , and the recovery of the drain-current is monitored from about 1 ms up to 12 s. After the last stress interval, the device is allowed to recover for 3000 s. The recorded drain-current is then converted to a  $V_{th}$  shift using an initial  $I_D - V_G$  curve (recorded only around the threshold voltage to avoid prestressing the device). Unfortunately, any measurement performed by interrupting the stress introduces an unavoidable delay and recovery effects faster than 1  $\mu$ s have eluded experimental effort [29], which is sometimes considered a drawback of this method. However, in contrast to OTF measurements, such a setup is much less prone to errors introduced by mobility variations [8] and determination of the initial drain-current  $I_{D0}$  [9] and the data consequently more reliable.

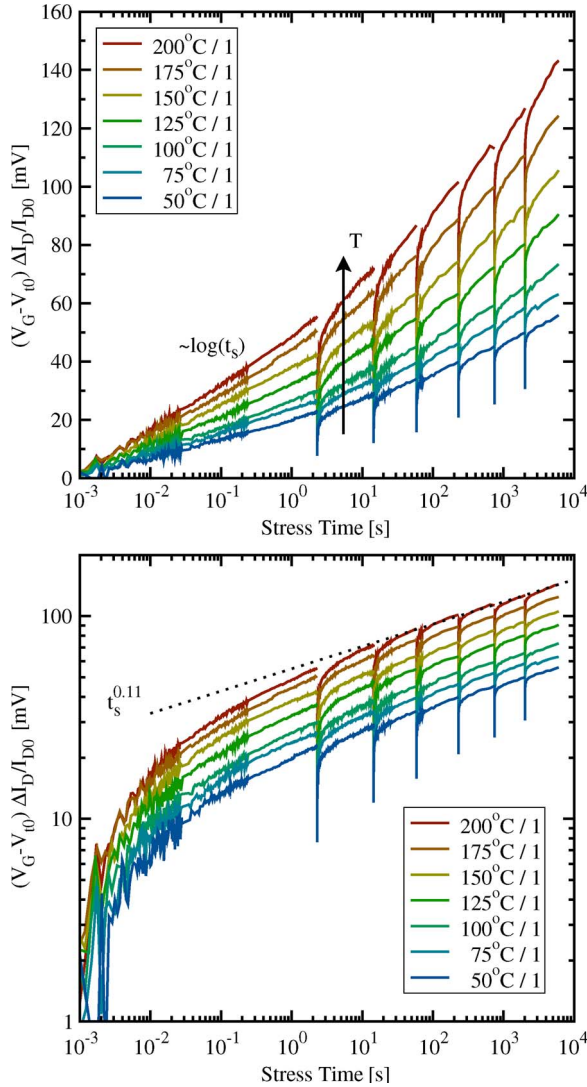


Fig. 1. Unscaled stress and restress phases of the eMSM measurement sequence on seven different devices at seven different temperatures (EOT = 1.4 nm,  $V_{\text{stress}} = -2$  V, and  $E_{\text{ox}} \approx 8$  MV/cm). Each stress interruption results in a recovery that appears to be quickly restored to the undisturbed level [7]. The initial degradation ( $t_s \lesssim 1$  s) follows a logarithmic time dependence while the long-time dependence resembles a power law with exponent  $n = 0.11$ .

The devices were stressed with voltages  $-1$ ,  $-1.2$ ,  $-1.4$ ,  $-1.6$ ,  $-1.8$ , and  $-2$  V at the temperatures of  $50^\circ\text{C}$ ,  $75^\circ\text{C}$ ,  $100^\circ\text{C}$ ,  $125^\circ\text{C}$ ,  $150^\circ\text{C}$ ,  $175^\circ\text{C}$ , and  $200^\circ\text{C}$ . P-channel field-effect transistors were used with  $W/L = 10\ \mu\text{m}/0.5\ \mu\text{m}$  and nitrided oxides fabricated using decoupled plasma nitridation into *in situ* steam-generated 1.64-nm-thick oxides. Postnitridation anneal in  $\text{O}_2$  resulted in a silicon oxynitride film with an equivalent oxide thickness (EOT) of 1.4 nm [25], [30].

### III. RESULTS AND DISCUSSION

The stress data obtained for the seven temperatures are shown in Fig. 1 on lin-log and log-log scales. As observed by other groups before [7], [9], [16], the initial degradation is log-like (straight lines on a lin-log plot roughly up to 1 s), followed by a power-law-like long-term behavior (straight lines on a log-log plot at longer stress times) with exponent  $n = 0.11$  (smaller than  $1/6$ ).

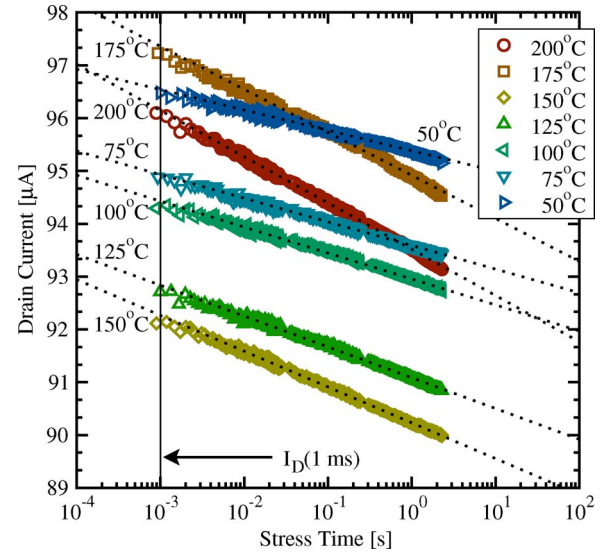


Fig. 2. Degradation of the absolute value of the drain-current at different temperatures upon application of a stress voltage of  $-2$  V (symbols). For the calculation of  $\Delta I_D(t_s) = I_D(t_s) - I_D(t_0)$ , the drain-current at  $t_0 = 1$  ms is required. Since this value has a strong impact on the whole analysis and is prone to noise, it is evaluated by fitting a logarithmic function to the data (lines). We remark that this function is only used for smoothing and not for extrapolation as in [28]. As a side note, we point out that the initial drain-current of the devices stressed at  $50^\circ\text{C}$ – $150^\circ\text{C}$  shows the expected temperature dependence, while the devices stressed at  $175^\circ\text{C}$  and  $200^\circ\text{C}$  have a larger initial drain-current. Interestingly, however, the relative change in  $I_D$  and, thus, the estimated  $\Delta V_{\text{th}}^{\text{OTF}}$ , of all devices follows the same pattern (cf. Fig. 1), indicating that the variation in initial  $I_D$  is due to device-to-device variations of a different origin.

In order to obtain  $\Delta V_{\text{th}}^{\text{OTF}}$  according to (3), a reliable determination of  $I_{D0} = I_D(t_0)$  is required. Ideally, the reference drain-current should be obtained at  $t_0 = 0$  s, which is, of course, impossible to obtain in practice because  $I_D$  already has to be measured at stress level [3], [9], [28]. While some reports claim that  $t_0 = 1\ \mu\text{s}$  may be fast enough [16], [23], others clearly show that the degradation of  $I_D$  is already in full flight at  $t_s = 1\ \mu\text{s}$  [28]. While this issue is probably difficult to resolve in a practical setup and may depend on the actual technology under consideration, we deliberately use  $t_0 = 1$  ms and take the thus calculated  $\Delta V_{\text{th}}^{\text{OTF}}$  as our OTF indicator for degradation. We must keep in mind, however, that this quantity may have different properties than a  $\Delta V_{\text{th}}^{\text{OTF}}$  calculated with  $t_0 = 0$  s.

Since the first measurement points are typically noisy, we determine  $I_D(t_0)$  more accurately by fitting a logarithmic function to the data in the interval [1 ms, 1 s]. In contrast to [28], however, we do not attempt to extrapolate the data to shorter times than those available in our measurements and use the fit only for smoothing purposes. This procedure is illustrated in Fig. 2.

In an attempt to separate the two distinct contributing mechanisms, we normalize the stress and restress data obtained from our eMSM measurement to a selected measurement (the least noisy one). A typical plot is shown in Fig. 3, where the data obtained at different temperatures from Fig. 1 are normalized to the  $50^\circ\text{C}$  data. Astonishingly, one observes that  $\Delta V_{\text{th}}^{\text{OTF}}$  is proportional to the  $50^\circ\text{C}$  data at all temperatures, in contradiction to the “two-independent-mechanisms hypothesis.” This

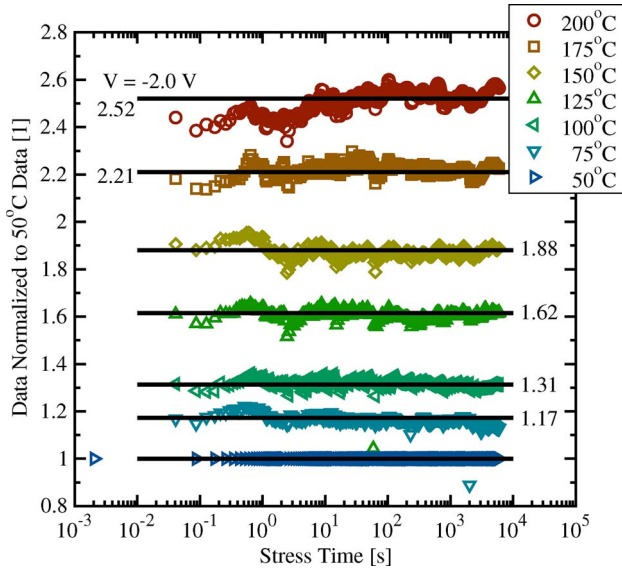


Fig. 3. Data of Fig. 1 (different temperatures with a stress bias of  $V_{\text{stress}} = -2$  V) normalized to the 50 °C data. The data differ only by a temperature-dependent prefactor. Due to the large noise in the initial data, only ratios for  $t_s > 40$  ms are shown. Prior to normalization the data was smoothed using the ACSplines algorithm as implemented in GNUPLLOT.

peculiarity is also demonstrated in Fig. 4, where the scaling factors obtained in Fig. 3 are used to make the data of Fig. 1 overlap perfectly.

As shown in Fig. 5, a similar scaling property is observed during recovery when normalizing the recovery data obtained in the eMSM measurement of Fig. 1 to the first recovery point of the last long recovery sequence. Although the data are somewhat noisy and device-to-device variations cannot be ruled out, it appears that the relative recovery slows down at higher temperatures, indicating a slightly larger “permanent” degradation [24], [31]. Interestingly, despite the different measurement techniques used during stress and recovery, the obtained scaling factors are in very good agreement.

A similar scaling property is observed for the voltage dependence, as shown in Figs. 6–8. While the voltage-dependent proportionality factor is well defined in Fig. 7, the behavior during recovery is slightly different. As shown in Fig. 9, a higher stress voltage results in a slower relative recovery.

Finally, all scaling factors collected during stress and recovery are summarized in Fig. 10. It is interesting that for both temperature and voltage scaling, the factors obtained during stress agree very well with those obtained during recovery.

We remark that the scalability of the OTF stress data has been reported for instance in [23] for certain plasma nitrided oxide devices and was explained as being characteristic for devices where the creation of interface states is dominant. As most likely explanation for this interface state creation, the RD mechanism was given. We remark here that neither the initial log-like degradation nor the log-like recovery can be explained by RD theory [32]. Rather, both the log-like initial degradation as well as the log-like recovery have been explained via a hole-trapping mechanism [3], [4], [32]. Thus, the fact that the scaling factors during initial log-like degradation, long-time stress, and recovery are basically the same is indeed remarkable.

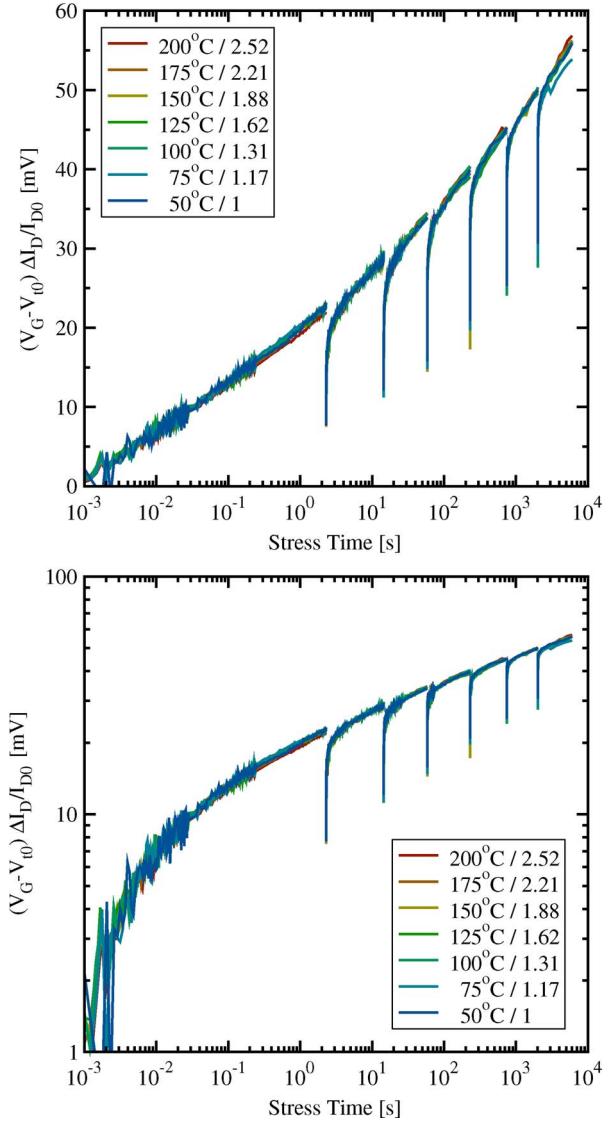


Fig. 4. Scaling of the data shown in Fig. 1 by the factor obtained in Fig. 3 results in a perfectly overlapping “universal” curve for all stress times investigated here. The scaling factors are given in the legend.

Figs. 3–10 clearly demonstrate that both voltage and temperature scaling with single multiplicative coefficients across all measured times and for both stress and relaxation phases is excellent. Hence, despite the fact that our data display all the ingredients that have been previously interpreted using two independent mechanisms, the observed scaling property strongly suggests that NBTI in our devices is driven by a single dominant or a tightly coupled mechanism and can, in good approximation, be empirically written as

$$\Delta V_{\text{th}}^{\text{OTF}}(t_s, T_{\text{stress}}, V_{\text{stress}}) = f(T_{\text{stress}}, V_{\text{stress}}) \Delta V_{\text{th}}^{\text{OTF}}(t_s, T_{\text{ref}}, V_{\text{ref}}) \quad (4)$$

with a temperature- and voltage-dependent scaling factor  $f$ .  $T_{\text{ref}}$  and  $V_{\text{ref}}$  are the temperature and voltage for a suitably chosen reference curve. The recovery data appear to be slightly more complicated, with a slowdown of recovery observed at larger stress voltages and temperatures.



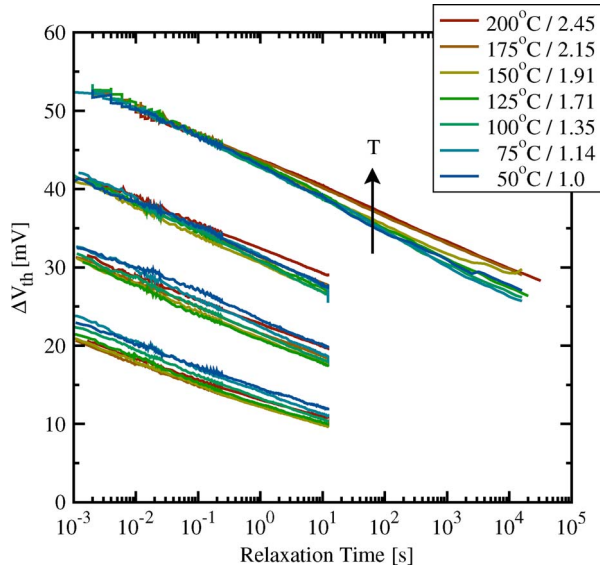


Fig. 5. Normalization of the data to the first recovery point of the last (long) recovery sequence results in similar scaling factors as those obtained in Fig. 3. The four different sets of recovery sequences belong to different stress times in the eMSM measurement. Although the effect seems to be small, the relative recovery appears to be slightly smaller for higher temperatures. Any such slowdown of the recovery may be counterbalanced to an unknown extent by the use of a temperature-dependent threshold voltage during recovery ( $V_{th}(50^\circ\text{C}) \approx 340\text{ mV}$  and  $V_{th}(200^\circ\text{C}) \approx 230\text{ mV}$ ).

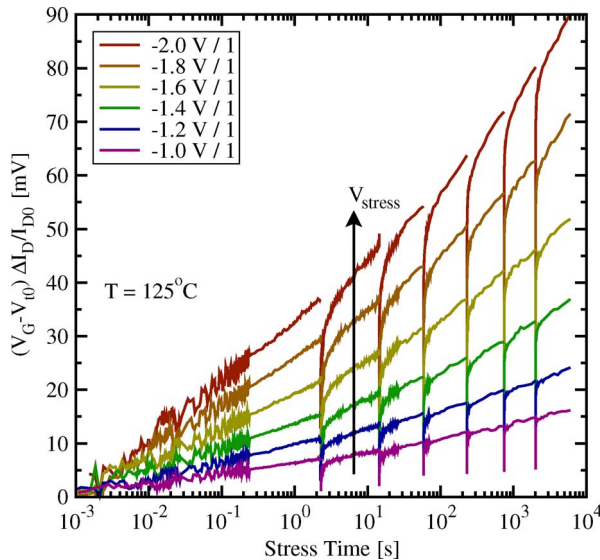


Fig. 6. Same eMSM sequence as in Fig. 1, but now for different stress voltages at  $T = 125^\circ\text{C}$ . Again, the initial logarithmic evolution depends strongly on the stress voltage.

If NBTI were driven by two *independent* mechanisms, the validity of (4) would be highly unlikely due to their expected different voltage and temperature dependences. Furthermore, the relation in (4) indicates that the NBTI mechanism is of a more complicated nature than previously suggested. In particular, the data appear to be consistent with two *coupled mechanisms* where the degradation occurs in two stages. An example that is compatible with the current understanding would be that in stage 1 holes are trapped, and these trapped holes then trigger the creation of defects in the second stage. We remark that depending on the process, this hole-trapping component may

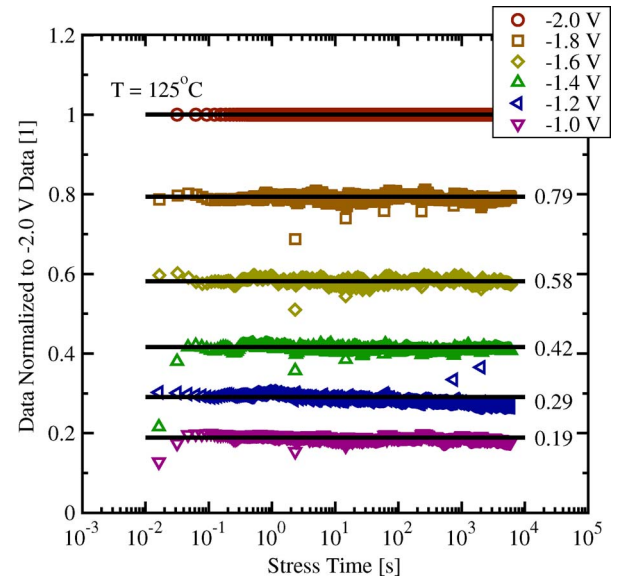


Fig. 7. Data of Fig. 6 scaled to  $V_{\text{stress}} = -2\text{ V}$  (least noisy data). Quite convincingly, the data scale nicely with the stress voltage.

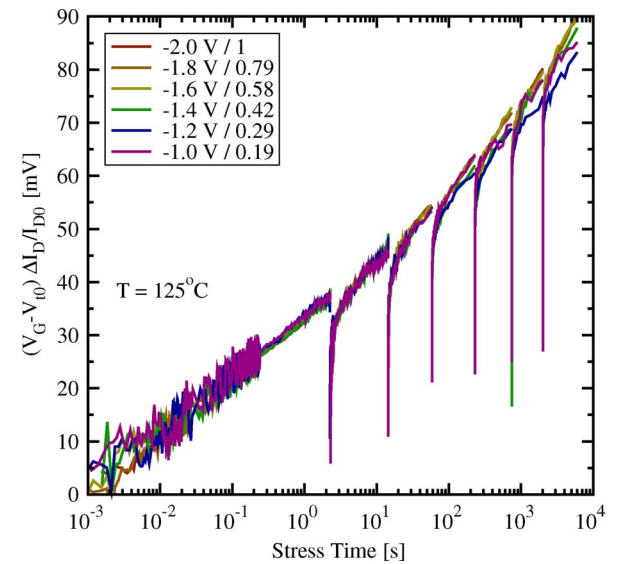


Fig. 8. Data of Fig. 6 scaled with the scaling factors obtained in Fig. 7, nearly perfectly overlap, regardless of the complicated stress/restress pattern. The data obtained at  $V_{\text{stress}} = -1.2\text{ V}$  are slightly different at long stress times.

saturate. In such a case, defect creation could continue, thereby making the coupling less obvious to observe. During recovery, our data indicate that the coupling of the two components may become weaker or may be even absent.

Note that a simple example of such a coupled process is also used in the RD theory where the forward rate for interface state creation is assumed to be proportional to the hole concentration in the inversion layer [18]. Nevertheless, in such a simple scenario, the hole trapping step is assumed to happen instantaneously and therefore does not contribute anything to the overall dynamics of the process, in contrast to claims raised in [14], and thus cannot explain the data (see [8]).

We finally remark that such a two-stage process has been previously suggested in the context of irradiation damage [33]: in the first stage, irradiation-induced holes are trapped in  $E'$

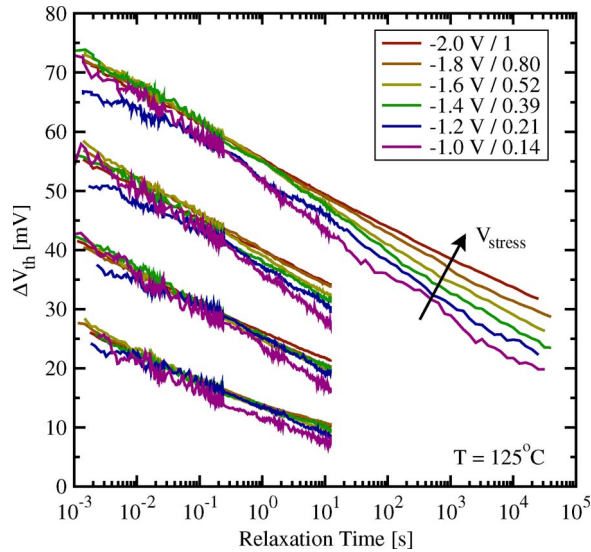


Fig. 9. Recovery data belonging to the stress sequences of the eMSM measurement of Fig. 6. As in Fig. 5, the data are scaled to the first recovery point of the last recovery sequence, except for the data obtained at  $V_{\text{stress}} = -1.2$  V, which again initially fall out of line. Overall, recovery seems to be slower for larger stress voltages. During recovery,  $V_{\text{relax}} = V_{\text{th}} = 300$  mV was used.

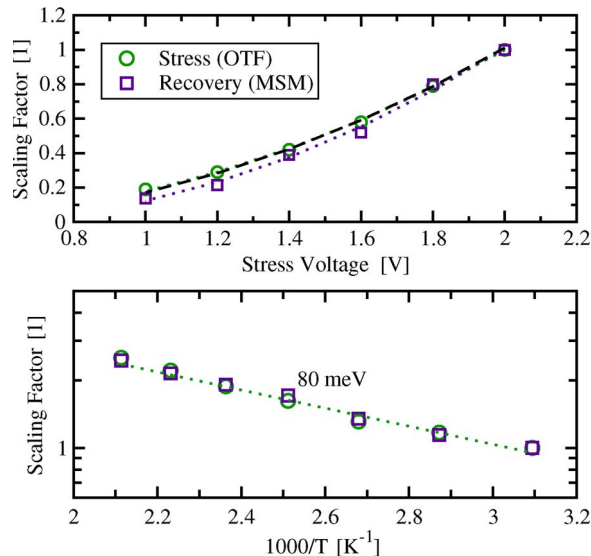


Fig. 10. Collected scaling factors as a function of  $V_{\text{stress}}$  and  $T$ . While the temperature dependence follows the Arrhenius law, the voltage dependence can be fit to the quadratic expression  $C_1(V_{\text{stress}} - C_2)^2$  (dotted lines) and in particular to  $0.35(V_{\text{stress}} - V_{\text{relax}})^2$  (dashed line) [26]. For the temperature dependence, the difference in the scaling factors obtained from the stress and the recovery data is within the experimental error, while the scaling factors for the voltage dependence obtained during stress and recovery show a somewhat larger deviation. Furthermore, the observed temperature activation of the scaling factors is within the range of activation energies observed by other groups [22], [23].

centers, thereby creating silicon dangling bonds next to the interface. In stage 2, based on basic thermodynamic arguments, the passivated dangling bonds at the interface loose their hydrogen to the newly created dangling bonds inside the oxide, thereby creating electrically active interface states. The data presented here clearly indicates that a similar mechanism is possible in the case of bias temperature instability [34].

#### IV. CONCLUSION

A growing number of recent publications discuss the possibility of two distinctly different mechanisms contributing to NBTI, namely, interface state generation and hole trapping. Evidence for that are the log-like initial degradation followed by a power-law-like long-term behavior and the log-like recovery on top of a permanent or very slowly relaxing component. Based on the notion that such different mechanisms are very likely to have different voltage and temperature dependences, one would expect that these different dependences would leave a distinct mark on the measurement data and allow one to at least partially separate their contribution to the overall degradation.

Consequently, we have performed NBTI stress and recovery measurements at different temperatures and voltages in order to investigate such a separability in our samples. Remarkably, although our data also show the previously suggested signatures of these two mechanisms, i.e., initial log-like degradation followed by a power-law-like degradation, the stress degradation data obtained at the investigated temperatures and voltages can be perfectly scaled to a universal form, making the contribution of two *independent* mechanisms highly unlikely. This is also approximately true during recovery, with higher temperatures and higher voltages resulting in a slight slowdown of recovery.

It is important to realize that the scaling factors obtained for the initial log-like degradation ( $t_s = 1$  ms–1 s) agree perfectly well with those obtained for longer stress times ( $t_s = 1$  s– $10^4$  s), making an explanation based on two *independent* mechanisms predominantly acting in one of these two regimes artificial.

Given our data, an explanation invoking only a single “all-encompassing” mechanism or two *coupled* mechanisms appears to be the most straightforward approach to understanding NBTI. This mechanism has to be more complicated than those previously suggested in order to explain the rich spectrum of experimentally observed features [32], [35]. Based on our current understanding of the phenomenon, we favor an explanation where hole trapping and defect creation act in a coupled fashion.

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