The Paradigm Shift in Understanding the Bias Temperature Instability: From Reaction–Diffusion to Switching Oxide Traps

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(Invited Paper)

***Abstract*—One of the most important degradation modes in CMOS technologies, the bias temperature instability (BTI) has been known since the 1960s. Already in early interpretations, charge trapping in the oxide was considered an important aspect of the degradation. In their 1977 paper, Jeppson and Svensson suggested a hydrogen-diffusion controlled mechanism for the creation of interface states. Their reaction–diffusion model subsequently became the dominant explanation of the phenomenon. While Jeppson and Svensson gave a preliminary study of the recovery of the degradation, this issue received only limited attention for many years. In the last decade, however, a large number of detailed recovery studies have been published, showing clearly that the reaction–diffusion mechanism is inconsistent with the data. As a consequence, the research focus shifted back toward charge trapping. Currently available advanced charge-trapping theories based on switching oxide traps are now able to explain the bulk of the experimental data. We give a review of our perspective on some selected developments in this area.**

***Index Terms*—Bias temperature instability, charge trapping, NBTI, oxide defects, PBTI, reaction–diffusion, stochastic variability, switching oxide traps, reliability.**

I. Introduction

JUDGING from the number of publications in recent journals and conference proceedings, the bias temperature instability (BTI) is among the most discussed and most controversial topics in modern reliability research. Two issues have dominated the discussion, i.e., how to properly measure the degradation and the identification of the microscopic origin behind the degradation. Starting from the first paper suggesting a hydrogen-diffusion controlled interface state creation mechanism back in 1977 [1], the bulk of literature appeared to be unanimously supportive of this reaction–diffusion (RD) theory until about 2006 [2]–[5]. Then, for a while, RD theory was assumed to be essentially correct, but hydrogen diffusion was suggested to be dispersive [6]–[12].

A break with the RD tradition was brought about by the work of Huard *et al.* [13], who suggested that negative BTI (NBTI) is due to a more or less permanent reaction-controlled interface state creation mechanism based on the ideas of Haggag *et al.* [14]. In addition, recoverable elastic hole trapping [15] was used to explain NBTI recovery. As a consequence, hole trapping has become a subject of debate, and its existence is by now universally acknowledged. Still, proponents of the RD theory consider hole trapping a mere experimental nuisance, which pollutes the initial experimental data up to 1 s and has to be removed to unveil the real (RD) degradation mechanism [16].

Quite to the contrary, based on a long list of experimental observations inconsistent with the RD theory, recent studies strongly suggest that hole trapping is the *dominant* contributor to the degradation [17]–[27]. Interestingly, this possibility was already suggested in the very first papers on BTI [28], including the pioneering paper on RD theory by Jeppson and Svensson [1].

Starting from a detailed list of the deficiencies of the RD theory, we will summarize recent efforts toward a charge-trapping-dominated theory. Although the experimental evidence discussed in this paper is focused on NBTI in pMOS transistors, recent studies indicate that the microscopic physics behind BTI is the same for nMOS and pMOS transistors with SiO_2, SiON, and high-κ dielectrics [29], [30].

II. Inadequacy of the Reaction–Diffusion Theory

From a historical point of view, it appears that the role of charge trapping was completely swept under the carpet by the apparent success of the RD theory. Indeed, when devices with SiO_2 and SiON oxides are subjected to constant bias stress,

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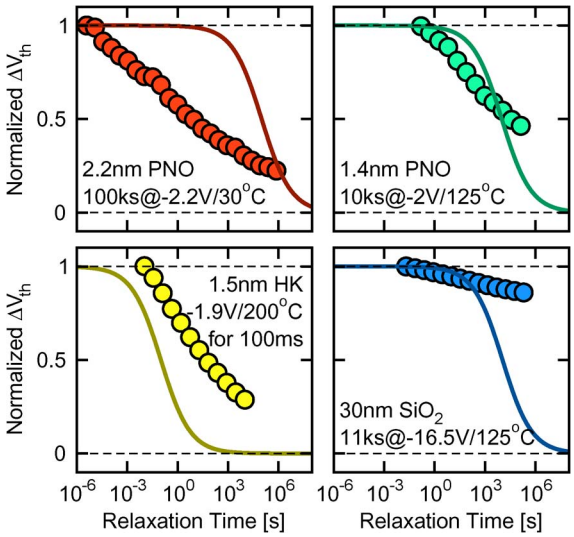

Fig. 1. Recovery at $V_G = V_{\rm th}$ for four different technologies always follows a $\log(t_r)$-like behavior. The symbols are data, and the lines are the RD prediction. RD recovery occurs dominantly over four decades in time, in stark contradiction to experimental data (Fig. 2).

the degradation as a function of time can be well captured [1], [3]–[5]. Only when researchers started to look at the detailed features of recovery, striking contradictions began to emerge [13], [18], [31], [32], which will be summarized here.

A. Nondispersive Reaction–Diffusion Models

The conventional RD theory predicts universal recovery, meaning that, when $\Delta V_{\rm th}$ is normalized to its value at the end of stress, it depends only on the ratio of the stress and relaxation times t_s and t_r [31]. In particular, in the dominant diffusion-limited phase, neither the forward nor backward reaction rates at the interface nor the (bias-independent) diffusion coefficient have any influence on the recovery. Approximately, normalized RD recovery can be written as [31]

$$\frac{\Delta V_{\rm th}(t_s,t_r)}{\Delta V_{\rm th}(t_s,0)} = \frac{1}{1+(t_r/t_s)^{1/2}}. \qquad (1)$$

This result is remarkable as it stands in stark contrast with experimental facts. One experimental fact is that recovery is already in full flight in measurements taken on the microseconds timescale [18], [33], independently of the stress time. This is inconsistent with (1), which predicts negligible recovery for $t_r \ll t_s$.

In an attempt to overcome this contradiction, the most recent versions of the RD theory postulate NBTI as being due to a superposition of elastic hole trapping, which saturates within about a second, followed by the "classic" H_2 diffusion-limited creation of interface states, which dominates degradation and recovery at longer times [16], [34].

However, during the last couple of years, evidence has piled up, which clearly demonstrates that NBTI recovery cannot be the diffusion-limited process suggested by the RD model.

1) The RD theory predicts a relatively short recovery phase lasting about four decades. In particular, a 50% recovery level is expected as soon as the relaxation time equals the stress time $t_r^{50\%} = t_s$. In addition, following a 10-ks stress, the RD theory predicts that only 1% of the degradation will have recovered in the first second. In reality, however, recovery is rather uniform and roughly follows $\log(t_r)$ over the whole experimental window (see Fig. 1). Recovery is already visible in the fastest measurements available (microsecond regime) and, after longer stress times, continues unabated [18]. In particular, saturation of the recovery is rarely observed [35].

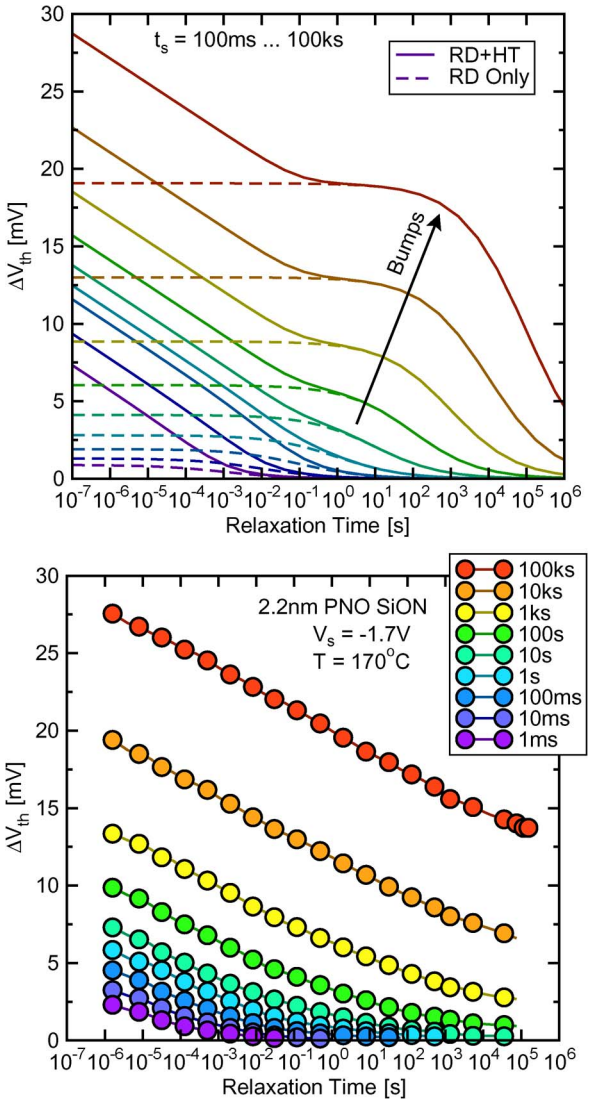

Fig. 2. Extended RD models with superpositioned hole-trapping result in discontinuous recovery traces (top), i.e., a "bump" is observed when RD recovery takes over from hole detrapping. This "bump" depends on the stress time and has never been observed experimentally (bottom). The bottom figure shows the evolution of typical "bump-free" experimental recovery traces with increasing stress times.

In an attempt to match RD recovery to experimental data, a virtual hole-trapping component was subtracted from the data in [34], leading to reasonable agreement for three decades, since only very short recovery times of up to 1 ks were considered. As shown in Fig. 2, however, experimental recovery stretches over many more decades before and after that time frame in a more-or-less uniform

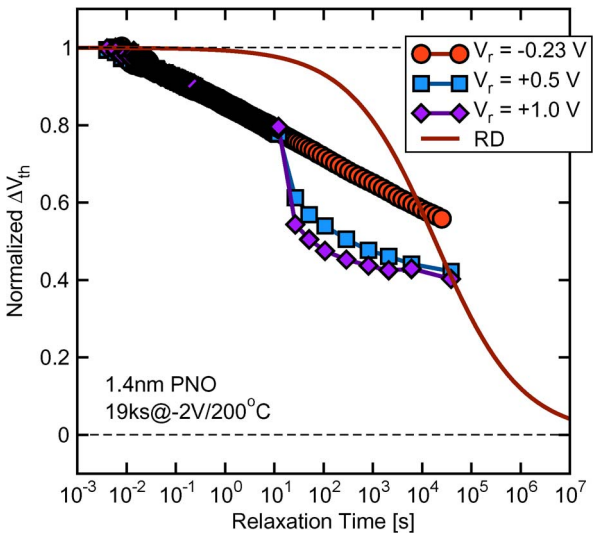

Fig. 3. Short switches to positive biases after 10 s of normal recovery at $V_G = V_{\rm th}$ considerably accelerate recovery. The RD model is based on neutral H_2 diffusion and, thus, oblivious to such bias changes.

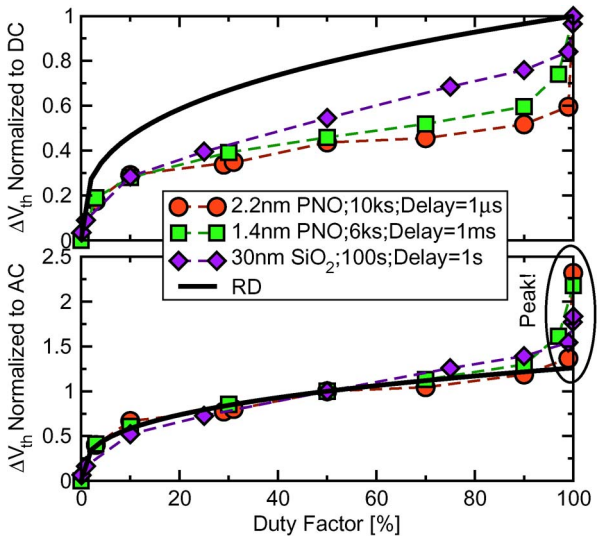

Fig. 4. DF dependence of the degradation for three different technologies. The RD model cannot reproduce the ubiquitous step shape, which sensitively depends on the measurement delay. Data are normalized to the (top) dc (DF = 100%) case and (bottom) ac (DF = 50%) case.

manner. Furthermore, the construction of the uniform experimental recovery trace using two disjunct processes leads to unnatural "bumps" in the recovery characteristics when more than a single stress time is considered (see Fig. 2). No such bumps have ever been observed experimentally.

2) RD-predicted recovery is due to the back diffusion of neutral H_2 and, as such, bias independent. In fact, however, experimental recovery is *strongly bias dependent* when V_G is switched toward accumulation. This bias dependence occurs well beyond the alleged saturation of the hole-trapping component of about 1 s and thus must be an intrinsic feature of the dominant recoverable component (see Fig. 3).
3) The duty-factor (DF)-dependent degradation predicted by the RD theory follows $\mathrm{DF}^{1/3}$, whereas, experimentally, a step-shaped curve is observed, with a very sharp drop of the degradation, even for small deviations from the ac case [25], [36], [37]. In particular, for DF = 50% (AC), RD predicts 80% of the dc degradation level, whereas experiments give a value typically smaller than 50% [see Fig. 4 (top)]. It has been recently suggested that the sharp increase for DF $\rightarrow$ 100% is due to the elastic hole-trapping component, whereas the main curve up to, e.g., DF $\approx$ 70%, is well covered by the RD theory [38]. The argument was supported by normalizing the degradation level to the ac rather than the dc value [see Fig. 4 (bottom)]. However, a closer look at the recovery time dependence of the step curve clearly reveals the problem of this argument (see Fig. 5): Although, with increasing recovery time, the peak at DF = 100% becomes smaller relative to the value at DF = 50%, the step shape does not go away, even after 30 ks of recovery. Any elastic hole-trapping component would long have vanished by this time in such a thin oxide. This again demonstrates that the peak at DF = 100% is an intrinsic part of the degradation rather than some experimental nuisance that can be arbitrarily removed.
4) Experimental recovery is independent of the hydrogen passivation degree of the interface (hydrogen budget) [22], [39], [40]. This is inconsistent with the idea that hydrogen back-diffusion controls recovery, as then the overall amount of hydrogen available next to the interface would surely have an impact [12]. For example, the RD theory predicts a considerable impact of the initial passivation degree of the interface states on the degradation behavior [12], contrary to experimental observations.

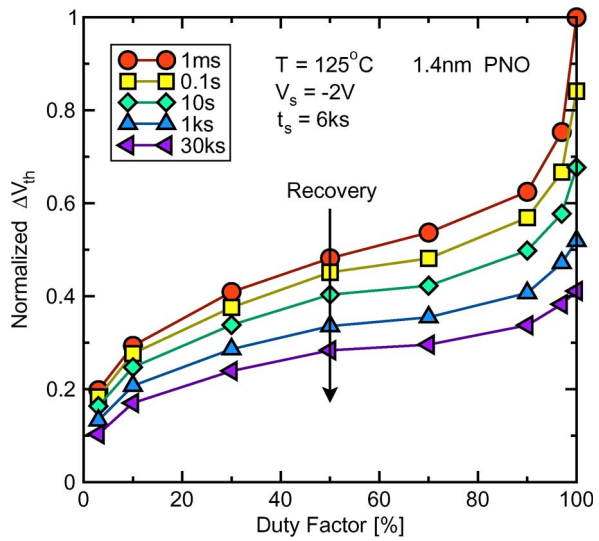

Fig. 5. DF dependence of the degradation normalized to the DF (100%) case with a delay of 1 ms. With increasing measurement delay, the degradation recovers. While the peak at DF = 100% (dc) shows as stronger recovery than the plateau at DF = 50% (ac), the basic features are not changed. This rules out that the peak at DF = 100% is due to elastic hole trapping, which would have to disappear after about 1 s in this thin oxide.

B. Reaction-Dispersive-Diffusion Models

From about 2005 to 2007 variants of the RD theory employing dispersive hydrogen transport were considered [6]–[8], [12]. In essence, these reaction-dispersive-diffusion (RDD) models use a time-dependent diffusivity $D = D_{00}(\nu t)^{\alpha-1}$, with ν being an attempt frequency, $\alpha = \mathrm{k}_B T_L/E_0$, and the characteristic energy E_0. While the details of the transport model appear to be of minor importance, the coupling to the interfacial reaction is essential [12] and divides the RDD models into two types: First, most models implicitly assume that all interfacial hydrogen, no matter how deeply trapped, is available for the passivation of dangling bonds [6]–[8]. This decreases the power-law slope during stress as the backward rate becomes more efficient. Furthermore, recovery is always *faster* than in the conventional RD model, thereby missing the long experimental recovery tails. Second, in more realistic models, only unbound hydrogen is allowed to passivate a dangling bond [12]. This increases the power-law slope during stress as it slows down the backward reaction. On the other hand, recovery will always be slower than in the RD model, that is, no significant recovery is predicted for $t_r \lesssim t_s$ [41]. In addition, all RDD models predict a temperature-dependent power-law slope during stress, inconsistent with recovery-free experimental data [16].

In one of our early attempts to explain both universal recovery and a wide distribution on the recovery time axis, we introduced a dispersive hole transport model coupled to a dispersive hydrogen transport model [31]. In the spirit of the day, the model consisted of a uniform charge injection step, followed by a dispersive redistribution of the trapped holes, where the hole trapping sites where assumed to be the dispersively diffusing hydrogen. While it has been realized that modern oxides are simply too thin to support a hydrogen diffusion front, necessitating the postulate that hydrogen mainly diffuses in the polysilicon gate contact [42], such an extension is clearly pointless for dispersive hole transport. Another argument against hydrogen diffusion in the polysilicon gate is the similarity of NBTI degradation in thin and thick oxides, including high-k gate stacks with metal gates.

As a consequence, no succesful RDD description of NBTI recovery has been published in literature. Still, the main lessons learned from RDD models is that the dispersion of the time constants is not a consequence of the diffusion process but must be inherently included in the initial charge trapping step. In summary, as the RD theory and its variants are clearly inconsistent with experimental facts, it must be abandoned and replaced by a better theory. Attempts in that direction are summarized here.

III. Link to Random Telegraph Noise

A detailed look under the hood of BTI degradation can be provided by studying small-area devices. By the term *small-area devices,* we refer to devices smaller than those usually used for NBTI testing but still routinely available, e.g., $W \times L = 100$ nm $\times$ 100 nm. Recovery in these devices proceeds in discrete steps (see Fig. 6), which are not consistent with a diffusion-limited process [43]. Rather, they are consistent with the emission of individual holes based on a first-order reaction-rate process [24], [43]–[48]. In fact, our understanding of NBTI received a considerable boost when it was realized that all the properties of these discrete steps are fully consistent with charge trapping observed in the context of random telegraph noise (RTN) and $1/f$ noise [21], [24]–[27], [43], [45]–[48]. As such, a standard $1/f$ noise model [49] already captures more features of NBTI recovery than the RD theory, including the $\log(t_r)$ recovery [21] and the DF dependence [25].

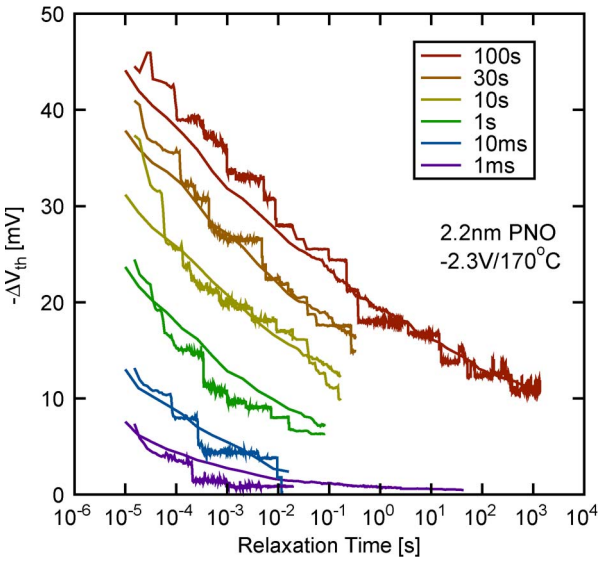

Fig. 6. Comparison of the recovery traces for a single narrow device (traces with steps) and the average over 25 different FETs (smooth traces) [25]. Each step is due to the discharge of a single hole. Emission events are equally distributed from the microsecond to the kilosecond regime. The averaged traces are very similar to recovery traces recorded on a large-area device, demonstrating that the discrete recovery steps are at the heart of the NBTI recovery phenomenon [25].

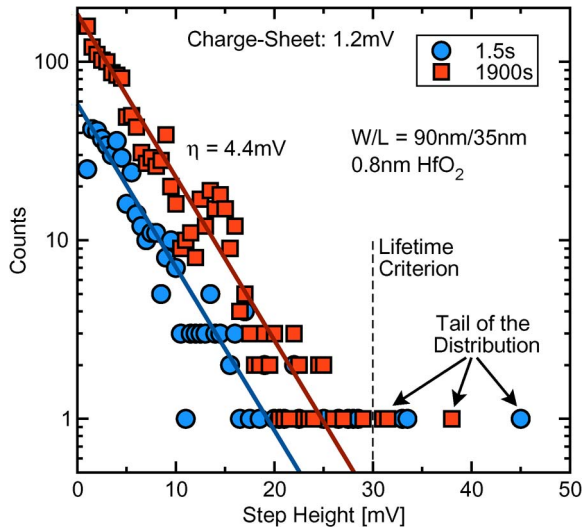

Fig. 7. Exponential distribution of step heights for two different stress times. Note that η is about four times larger than the charge-sheet value [27]. Even for short stress times, defects from the tail of the exponential distribution can produce threshold voltage shifts larger than 30 mV, which is a typical lifetime value.

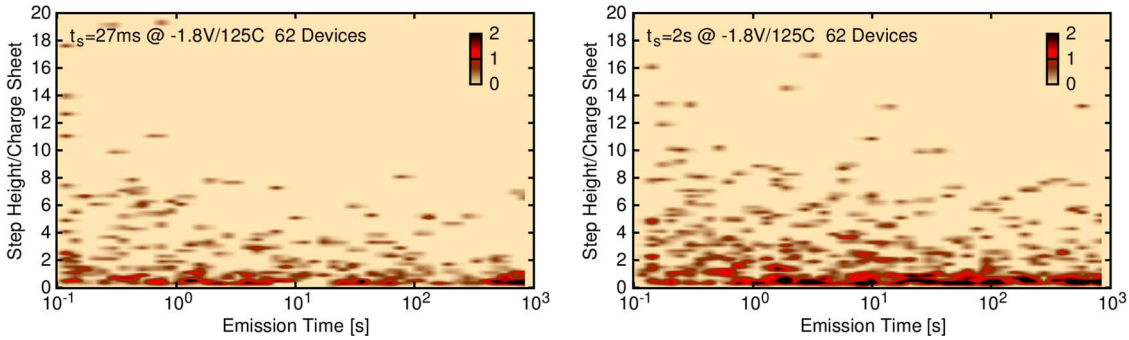

Fig. 8. Normalized step heights (0.6 mV) versus emission time after a stress time of 27 ms and 2 s. Even after a 27-ms stress, emission events with 1 ks are generated. With increasing stress time, the number of emission events is homogeneously increased over the whole emission time axis.

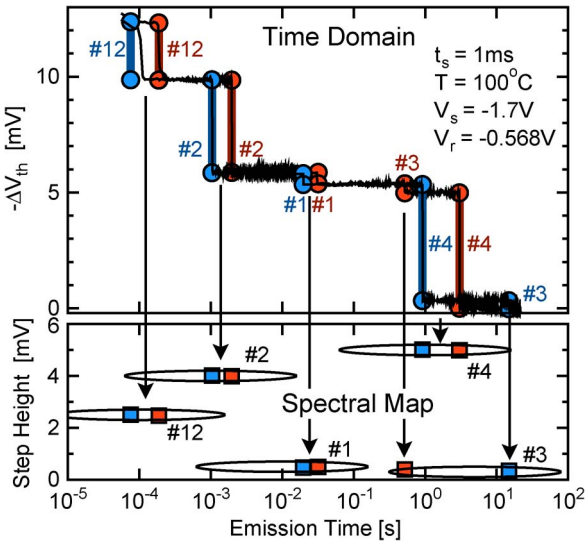

Fig. 9. (Top) The measured data are given by the noisy black lines. The thick blue and red lines, together with the symbols, mark the emission times and step heights, which are unambiguous fingerprints of each defect. (Bottom) Each step height/emission time pair is collect in the spectral map. With repeated experiments, clearly visible clusters form, which allow for a clear identification of the various defects.

Just like in RTN, the step heights can be considerably larger than expected from the simple charge-sheet approximation. This is a consequence of the random locations of the discrete dopants in the channel [50]. The step heights are exponentially distributed [27], [51] (see Fig. 7). This results in a nonnegligible probability that defects have step heights well beyond 30 mV in deeply scaled devices, which is a typical lifetime criterion. Even for short stress times, emission events with emission times $10^5\times$ larger than the stress time are observed and homogeneously distributed over the logarithmic time axis (see Fig. 8).

The recently developed *time-dependent defect spectroscopy* (TDDS, see Figs. 9 and 10) allows for the analysis of these steps as a function of stress/recovery bias conditions and temperature [24], [25], [52] and has revealed a number of interesting facts about the hole-trapping component.

1) Both capture and emission time constants are strongly temperature dependent, with activation energies around 0.5–1 eV. No defects with temperature-independent capture time constants—hinting at the elastic tunneling process invoked by the extended RD model—could be found in the experimental window covering the microsecond up to the kilosecond regime. This has been recently confirmed to be the same for positive BTI (PBTI) in nFETs [53] and PBTI/NBTI in high-κ FETs [29], [30].
2) The capture time constants show a very strong bias dependence. On the other hand, the bias dependence of the emission time constants around $V_{\rm th}$ may be either weak or strong, depending on the configuration of the defect. In order to explain this strong bias dependence, a metastable defect state must be considered in the model (see Section IV).
3) Charge capture is dominated by preexisting defect precursors, which could be, for example, oxygen vacancies [21]. For short stress times, the charging process is fully reversible, whereas, at larger stress times, defect transformation may occur [21], [24], [35], [54].
4) Metastable states are apparent in disappearing defects, anomalous RTN, and temporary RTN (cf. Fig. 11). Furthermore, the metastable states are required to explain the unexpected bias dependencies of the time constants [24].

In conclusion, the defects responsible for the recoverable component of BTI are identical to those causing RTN. Conceptually, the difference is given as follows: in an RTN experiment, only a limited number of defects having capture and emission time constants within the experimental window are visible. Due to the strong bias dependence of the capture time constant, many more defects contribute to BTI. Consequently, NBTI can be considered the nonequilibrium response of these defects, whereas RTN is a consequence of their quasi-stationary behavior [27].

IV. Charge-Trapping Mechanism

All these results clearly demonstrate the central role of charge trapping in NBTI [17], [20], [21], [24], [25], [43], [44], [46], [47], which is in line with the standard interpretation of PBTI in high-κ devices [55]–[57]. However, the usual theory invoked to explain such phenomena is due to McWhorter [58], who attributed the wide dispersion in the capture and emission time constants required to explain RTN and $1/f$ noise to defects located at various *depths* into the oxide. While it has been realized early on that elastic tunneling is unable to explain the universally observed strong temperature and bias dependence of the capture time constant [49], [59], [60], Campbell *et al.* [61]

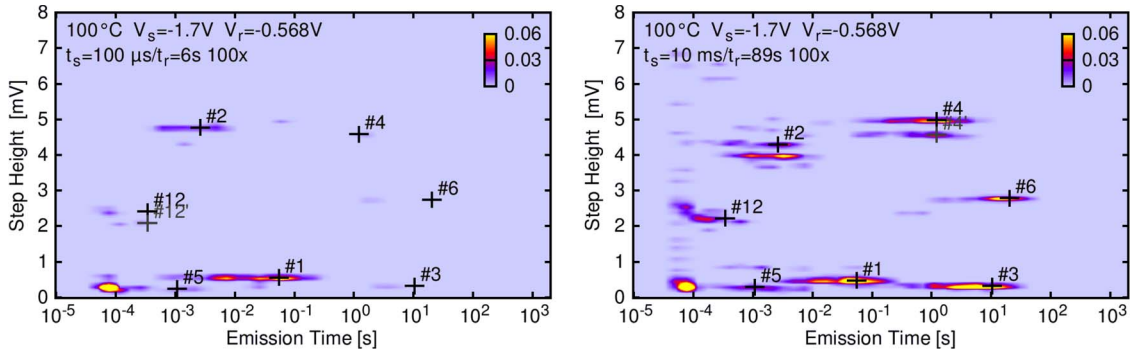

Fig. 10. Two TDDS spectral maps at two stress times (left) $t_s = 100\ \mu$s and (right) $t_s = 10$ ms. With increasing stress time, the number of defects in the map increases. The width of each cluster is given by the exponential distribution of τ_e (considered on a logscale), and the extracted defects/clusters are marked by "+."

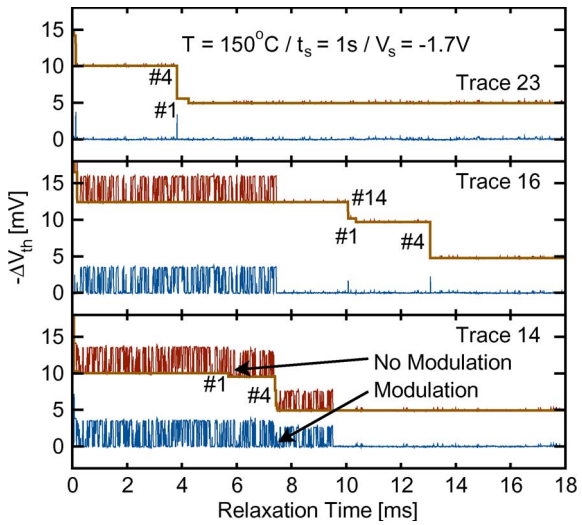

Fig. 11. In addition to the discrete recovery steps, the traces can contain temporary RTN (tRTN), which disappears after a certain amount of time (see the three selected traces). (Brown) The extracted step heights are subtracted from (red) raw data to yield (blue) the noise trace.

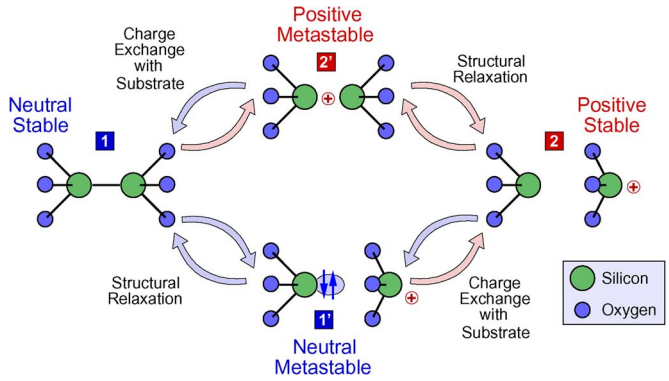

Fig. 12. Four states of the defect as extracted from the experimental data [24]. The defect is modeled around reported properties of the E' center.

explicitly demonstrated that *modern oxides are simply too thin* to support any significant distribution of time constants based on distance alone. Another confirmation of this fact has recently been given by Nagumo *et al.* [62], who demonstrated that the depth of the defect is uncorrelated with the characteristic time constants.

Thus, *rather than an elastic tunneling* process, *inelastic processes* have been applied to explain BTI data. The most consistent explanation is provided by the nonradiative multiphonon (NMP) theory [49], [63]–[65], which has recently been applied to BTI data [24]. In NMP theory, charge capture and emission is only possible when the sum of the electronic and vibrational energies of the defect is conserved. *Conservation of this total energy* introduces thermal barriers into the charge exchange process, thereby explaining the temperature dependence with the relatively large activation energies around 1 eV. In addition, since the electronic contribution to the total energy is either due to an electron at the defect site or in the substrate, application of an electric field leads to a strong bias dependence of these thermal barriers [24], [66].

Based on the standard model for E' centers developed in the context of irradiation damage [67], [68], we have suggested a defect model that is consistent with the experimental NBTI data [21] (see Fig. 12). The essence of this defect model is that, once the defect is created, its charge state can repeatedly change, depending on its energetic level in the band gap. As this is in contrast to trapped holes, which are not sensitive to bias changes, such defects are known as *switching traps*.

The extended model also allows for the description of various anomalies observed in the spectral map obtained by the TDDS. Depending on the defect potential energy surfaces, which are different for each defect in the amorphous oxide (see Fig. 13), the defect will show a different behavior when monitored under constant bias (RTN) or dynamic bias conditions (BTI).

1) In order to explain the large difference between capture and emission times, as well as the extremely strong bias dependence, which does not perfectly follow an exponential dependence, a positive metastable state $2'$ was introduced [24]. An example of the model fit to two typical defects is shown in Figs. 14 and 15.
2) Defects can disappear from the spectral map for random amounts of time, with the inactive defect being electrically neutral. This implies that such a defect has an electrically neutral metastable state.
3) A small number of defects produce temporary RTN (tRTN) after having been positively charged (cf. Fig. 11).

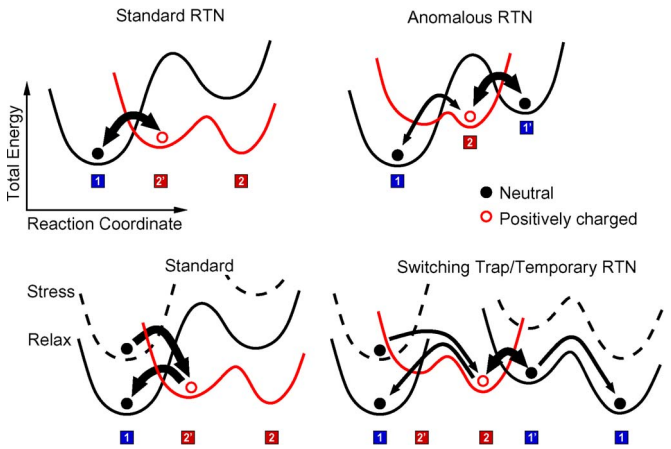

Fig. 13. Schematic configuration coordinate (CC) diagram model for a general defect [24]. In an amorphous oxide, each defect will have different configurational potentials that determine the NMP process. Depending on the bias conditions, the relative position of the potentials changes, causing a strong field dependence of the transition rates [66]. Thicker arrows indicate larger transition probabilities.

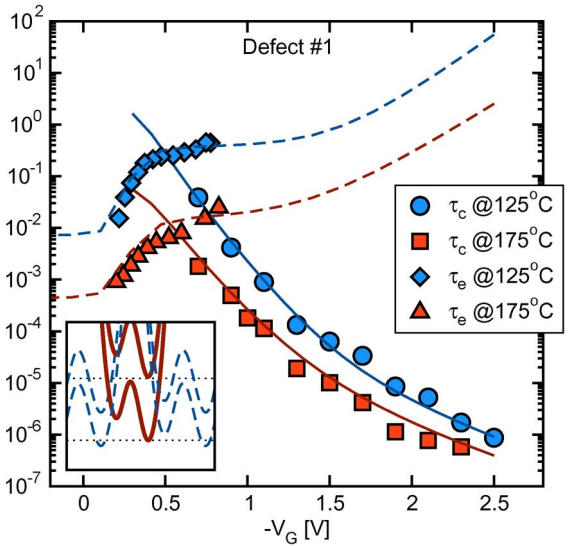

Fig. 14. Simulated capture and emission time constants for defect 1 of Fig. 10, compared to the experimental values. The CC diagram shown in the inset determines the switching trap behavior, where, for small V_G, defect annealing via the neutral metastable state is favored, resulting in a dramatic drop of the emission time constant.

This implies that the defect switches back and forth between its positive and metastable neutral state prior to annealing. These switches cannot be explained by transitions between the positive and the neutral precursor state, as the associated capture time constant is relatively large, particularly at low bias. This tRTN corresponds to the anomalous RTN under constant bias observed previously in standard RTN experiments [69].

4) The emission times of some defects show a very strong bias dependence for $|V_G| < |V_{\rm th}|$ (see Fig. 14). This is explained by a transition of the dominant recovery path over an alternative neutral metastable state [24].

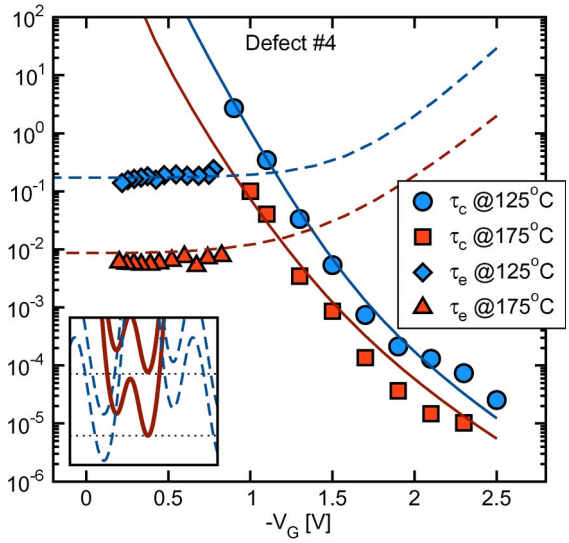

Fig. 15. In contrast to defect 1 in Fig. 14, the neutral metastable minimum of defect 4 is too high to be significantly populated, and no switching trap behavior can be observed. This can be clearly seen in the CC diagram shown in the inset. As a consequence, the emission time constant is insensitive to the gate bias, even for small V_G.

V. "Permanent" Component of NBTI

In order to explain their experimental data, Hurad *et al.* [13] separated the NBTI degradation into a recoverable and a permanent component R and P. Such a strategy was also successful in an empirical attempt, where we exploited the universal nature of R [37], [70], [71]. As shown in Fig. 2, however, R obviously dominates NBTI over the whole feasible experimental window, starting from the microseconds regime lasting many days or even months. As such, the characterization of P appears difficult [35] as there are no clear indications of P in the $\Delta V_{\rm th}$ recovery trace. In terms of the empirical universal extraction scheme, this resulted in unstable values for P, which tended to be close to the last measured $\Delta V_{\rm th}$ value. Hence, longer measurements resulted in smaller values of P, which is a clearly unsatisfying situation.

Since P cannot be feasibly extracted from $\Delta V_{\rm th}$ measurements, Huard *et al.* proposed that the permanent component is dominantly visible in the charge-pumping current $I_{\rm CP}$. However, this view is inconsistent with the data presented by Rangan *et al.* [72], who showed a strong recovery of $\Delta I_{\rm CP}$. Furthermore, it was demonstrated that the complete NBTI degradation can be annealed by increasing the temperature to 300 °C [22], [73], [74], which is not much larger than the usual NBTI characterization temperature of 200 °C. This confirms that the "recovery of the permanent component" is, just like the recovery of R, a thermally activated process. As a consequence, the separation into R and P is largely arbitrary based on electrical data alone. Hope exists though that electron spin resonance (ESR) measurements will eventually bring light into the matter whether R and P are due to different microscopic defects or merely a consequence of the wide distribution of time constants of a single or two coupled components (see Section VIII).

In favor of the latter option, which explains R and P by a single or two coupled components, we have observed that

oxide defects do not only dominate R and, thus, $\Delta V_{\rm th}$ but also contribute to $\Delta I_{\rm CP}$ and, therefore, P [35]. This contribution is significant and depends on temperature and frequency. In order to explain the larger time constants associated with P in comparison to R, the defect would have to undergo a transformation over metastable states. This defect transformation appears to be fully reversible.

Overall, the true nature of the link between R and P remains mysterious for the time being, and further studies are required [22], [35], [75], [76]. Still, even though not fully permanent, it appears useful to retain the expression "permanent component" to signify that fraction of the degradation with time constants outside the conventional measurement window.

VI. Two-Stage Model for NBTI

A first model able to capture a large number of the features discussed previously was suggested recently [21]. The degradation is assumed to proceed in two coupled stages. For the first stage, a simplified version of the defect model shown in Fig. 12 without the metastable positive state $2'$ was employed. The two-stage model thus assumes that charge is trapped in an E' center, thereby creating a switching trap.[1] Once charge is trapped in the defect, it is assumed that, via hydrogen exchange with a P_b center at the interface, the defect can transform into a more permanent state P. Although this coupling between E' and P_b centers is consistent with previous reports in the literature (see references in [21]), this assignment is still circumstantial.

The two-stage model is evaluated against some crucial NBTI benchmarks in Figs. 16–18. The experimentally observed behavior is fully reproduced, be it the asymmetry between stress and relaxation, the acceleration of recovery after positive bias pulses, or rapid switches in the temperature. For a discussion of the DF dependence, see [25].

Of particular importance is the dependence of the recovery on positive bias pulses, as shown in Fig. 17: in a standard two-state defect model, when the defect level is lowered below the Fermi level, hole emission from the defect will be *bias independent*, as the holes simply "bubble up." In our multistate defect model, defect annealing can proceed via the neutral metastable charge state. As a consequence, when the defect is positively charged, e.g., around the threshold voltage, recovery is inhibited. Quite to the contrary, when the defect is electrically neutralized by switching to positive biases, it has a much higher probability of being annealed (see Fig. 14 for the single-defect response and Fig. 17 for the multidefect response). As such, this multistate model can explain the density of states introduced in the band gap.

In other words, the main conclusion from the preceeding discussion is that positive charge is not just simply stored in the oxide, but injection of positive charge leads to the activation of a defect. This defect can be charged and discharged, and anneals preferably from its neutral metastable state.

[1]The transition rates used in [21] were phenomenological extensions of the NMP theory and should be replaced by the more rigorous NMP rates of [24].

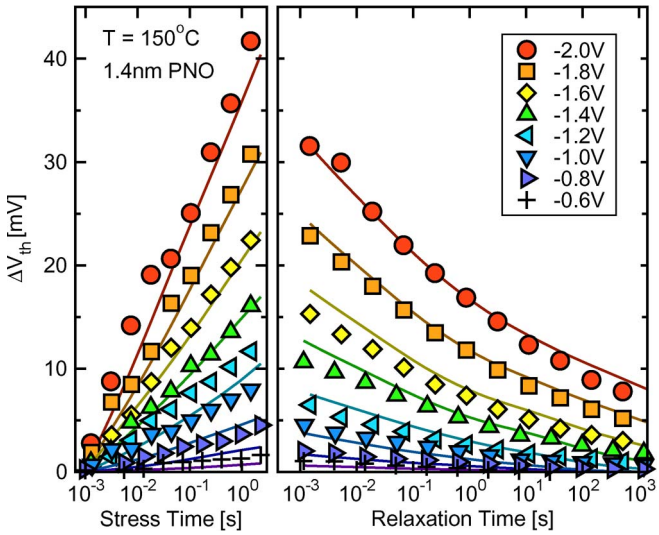

Fig. 16. A recently developed two-stage model [21] can already explain a number of crucial features of NBTI: Stress and recovery are asymmetric, with recovery taking much longer than degradation, and shown at 150 °C for eight different stress voltages for the 1.4-nm SiON devices. The asymmetry is properly reproduced by the model, resulting in a good fit during *both* stress and recovery.

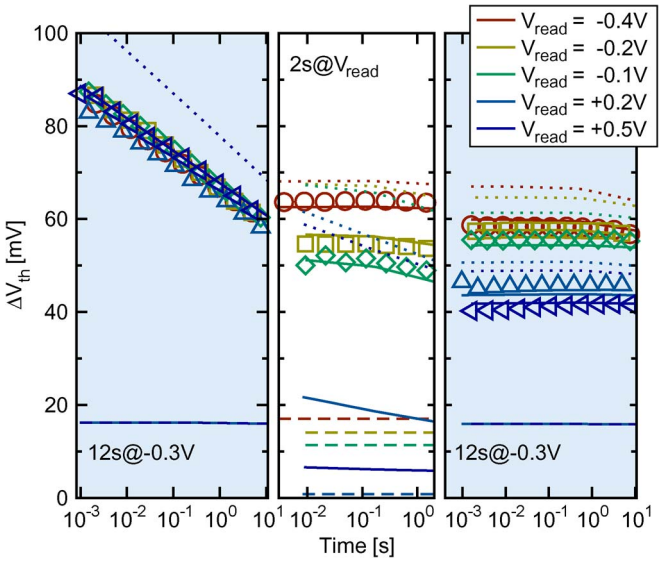

Fig. 17. Five devices were brought to the same level of degradation ($t_s = 6000$ s, $T = 125$ °C, $V_s = -2$ V). First, recovery was monitored for 10 s at $V_G = V_{\rm th} = -0.3$ V (panel 1). Then, the gate voltage was switched for 2 s to five different values, including more negative and more positive values (panel 2). When possible ($V_G < 0$ V), the change in the drain current was converted to $\Delta V_{\rm th}(V_G)$, which was found to be clearly different from $\Delta V_{\rm th}$ recorded at $V_{\rm th}$. Finally, V_G was switched back to $V_{\rm th}$ (panel 3), where a clear impact of the intermediate bias switch is observed. Simulation results are given by the lines (solid: positive defects (state 2), dotted: positive+neutral defects (states 2 and $1'$), dashed: permanent component), which show very good agreement with the data, capturing both the occupancy effect (panel 2) and the acceleration/retardation of recovery as a response to the gate bias (panel 3).

While the rates and states of the defect associated with R have been studied in great detail [24], the suggested transition rates regarding P [21] must be considered a first guess. Furthermore, since the model is based on $\Delta V_{\rm th}$ data, where P is only indirectly visible, it suffers from similar issues as those observed in the universal relaxation scheme. For example,

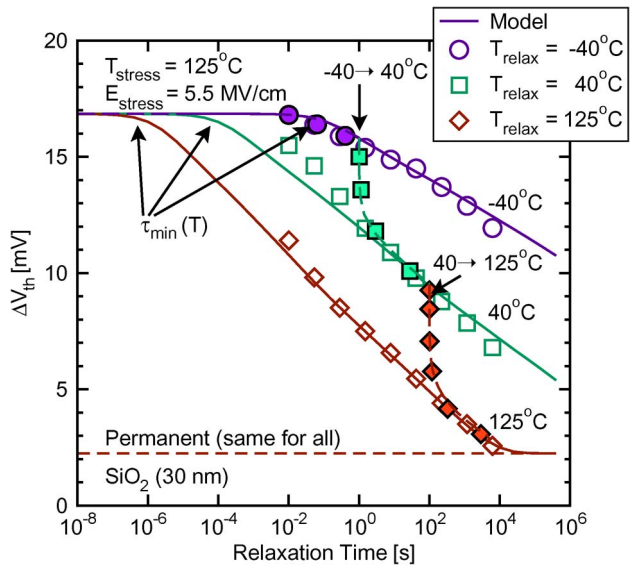

Fig. 18. Application of a recently developed polyheater technique [77], where a resistive structure locally heats the device and allows for high-precision switching of the device temperature within 1 s. Identically processed devices were stressed for the same time at 125 °C, whereas, prior to recovery, the temperature was quickly switched to −40 °C or +40 °C (open symbols). Finally, in a fourth device, the temperature was first switched to −40 °C; then, after 1-s recovery, to +40 °C; and finally, after 100 s, to 125 °C (filled symbols). Excellent agreement of the model with data is again obtained.

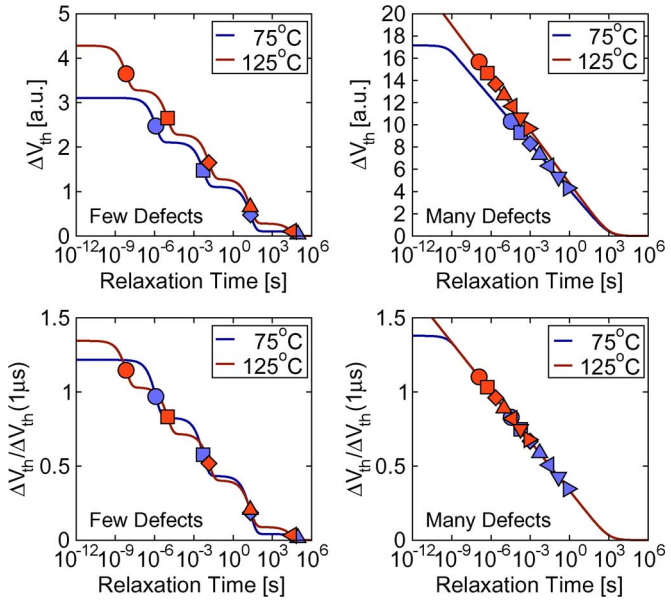

Fig. 19. In small-area devices with only a few active defects (left), the temperature dependence in the recovery remains visible after scaling the traces at some t_r time, e.g., the first measurement taken at 1 μs. Each symbol corresponds to a single defect and is located at the expectation value of the emission time, whereas the lines are a superposition of the individual transition probabilities. In large-area devices (right), the individual transitions overlap too much to be visible. Therefore, a defect with a higher activation energy seamlessly takes the place of a defect with a lower activation energy, resulting in an *apparent* temperature-independent behavior [25], [77].

the calibrated value of P shown in Fig. 18 is close to the last recorded $\Delta V_{\rm th}$ value and would certainly be lower if $\Delta V_{\rm th}$ had been measured for a longer time.

VII. Microscopic Versus Macroscopic Temperature Activation

At first glance, the present model with its thermally activated NMP processes appears to be at odds with the occasionally observed temperature independence of degradation and recovery [16], [18], [34]. Such a temperature independence is obtained when the $\Delta V_{\rm th}$ and $\Delta I_{\rm CP}$ recovery data are normalized to the first measured value [54]. However, this temperature independence is an artifact related to the relatively homogeneous density of states, which is an illusion thus visible only in the macroscopic response of large-area devices (see Fig. 19).

Similar conclusions hold for on-the-fly measurements [33]. There, the degradation of the drain current is measured relative to the first measurement point, which was taken for instance at 1 μs. In a hypothetical scenario where all defects have the same activation energy, the window of observable defects is simply shifted to shorter times at higher temperatures, whereas the number of defects stays the same. Thus, even with large individual activation energies, a temperature-independent degradation would be observed in large-area devices. In reality, the activation energies of the defects are only approximately uniformly distributed, resulting in a small overall macroscopic activation energy (0.1 eV), which is thus considerably smaller than the "physical" microscopic activation energies of the individual defects (0.5–1.2 eV) [24], [25]. As a consequence, great care has to be taken during the extraction of meaningful microscopic activation energies from such macroscopic measurements [25], [26].

VIII. Microscopic Nature of the Defects

Most studies on BTI are based on electrical data, which provide no information on the microscopic nature of the defects. The most promising techniques with the power to identify the microscopic nature of defects employ some kind of ESR technique. What is known from these ESR studies is that E' and P_b centers are created during NBTI stress. Furthermore, in devices with SiON gates, K_N centers have been identified [78]. Unfortunately, ESR measurements are notoriously slow and cannot be directly applied to fully processed MOSFETs, which are too small and have conductive layers in their gate stacks, obscuring the desired signals. To circumvent this problem, Campbell *et al.* [78] employed a spin-dependent recombination (SDR) technique, which showed a dominant P_b center signal. While this appears at odds with our model, one must keep in mind that the SDR experiments conducted in [78] favor efficient recombination centers around the middle of the band gap. The E' centers used in our model, however, have a very wide spectrum of time constants, and therefore, only a small fraction will be efficient recombination centers. In addition, if E' centers are responsible for R, a considerable amount would have recovered, even before the start of the measurement according to Fig. 2 (bottom). Altogether, one would thus reasonably expect a small concentration of E' centers, even when "the hell was beaten out of the devices" [79]. In a recent attempt to look especially for E' centers, an ESR measurement was conducted

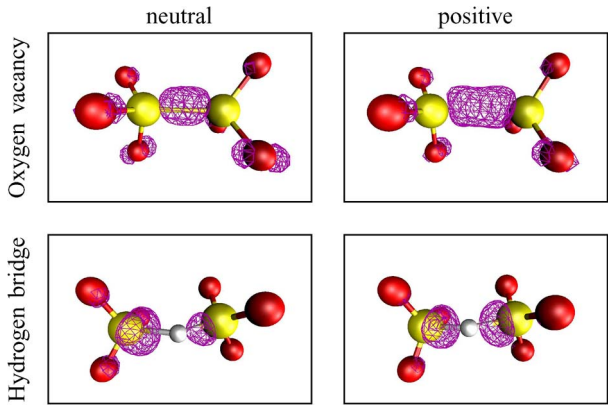

Fig. 20. Oxygen vacancy (top) and the hydrogen bridge in their optimized neutral and the positive charge states. The electron density obtained from DFT calculations is shown as a purple wireframe [80].

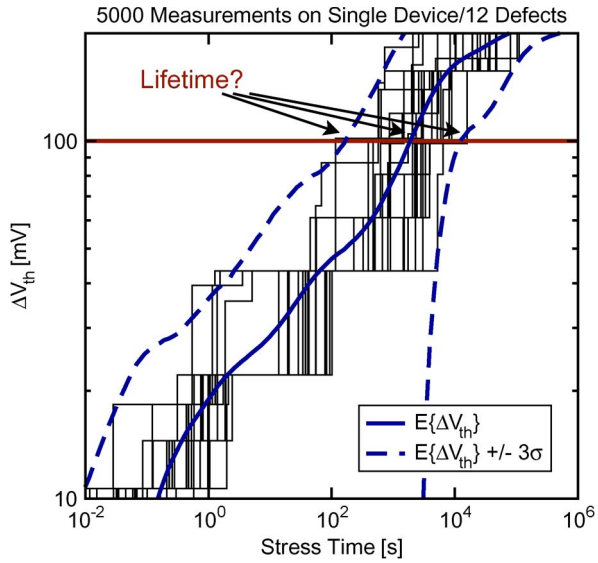

Fig. 21. Simulated repetitive degradation measurements on the *same* small-area device containing 12 defects give different results for each run due to the stochastic nature of charge trapping (thin lines). As a consequence, the *lifetime becomes a stochastic variable*. When the $\pm 3\sigma$ band (dashed lines) around the expectation value is considered (thick lines), the lifetime is reduced by about one order of magnitude.

on especially fabricated large-area devices under bias in an on-the-fly manner [75]. This ensures that the E' centers remain positively charged, thereby paramagnetic and visible in ESR. It also avoids recovery and does not favor effective recombination centers. The latter is insofar of importance as only a small fraction of the total number of defects contributing to the overall $\Delta V_{\rm th}$ shift may be effective recombination centers. Despite the considerable experimental difficulties, this study demonstrated the creation of a considerable amount of E' centers during stress. Consistent with the previous studies, the E' center signal rapidly disappeared after removal of the stress condition. One could expect that a large fraction of these disappeared E' centers are rechargeable by a small switch to more negative biases, which would be similar to what has been observed in ESR studies on switching oxide traps created by irradiation [68].

IX. Theoretical Defect Properties

Whereas our defect model is based on various reported properties of E' and P_b centers, a precise assignment is circumstantial. However, despite the fact that these defects are the most prevalent and thus most commonly studied defects in SiO_2 and related oxides, particularly, the E' center shows a number of features consistent with the TDDS data. Most prominent is the existence of metastable states, which could correspond to the puckered state of the positively charged E' center (the E'_γ center, state 2 in Fig. 12). A close relative of the E' center, which has already been suggested to be responsible for trap-assisted tunneling, is the hydrogen bridge [81]. Both defect structures are shown in Fig. 20 in their neutral and positive charge states.

In order to better understand the role of possible defect configurations, density functional theory (DFT) calculations could provide essential clues. While there exists a large body of literature dealing with the theoretical properties of the E' and P_b centers, the actual charge exchange mechanism with the substrate is rarely considered in sufficient detail. Furthermore, a number of issues make DFT studies of such defects challenging: First, the microscopic structure (the exact arrangement of the Si and O atoms) of an amorphous Si/SiO_2 interfacial layer is essentially unknown but a fundamental requirement for the correctness of the simulation. Second, the impact of the electric field is difficult to incorporate correctly. Finally, the DFT defect levels are notoriously difficult to align with reservoir levels, e.g., the conduction or valence level [82]. The situation becomes even more complex when the defect levels of an SiO_2-bulk structure have to be referenced to the silicon valence level of a metal–oxide–semiconductor structure. As such, a comparison of relaxation energies obtained from bulk structures [83] can only be a first step, and a considerable amount of work remains to be done in order to unambiguously identify the responsible defects [80].

X. Stochastic Lifetimes

During conventional reliability benchmarking, the degradation of devices is monitored under the assumption that their behavior is representative for all other devices. However, as is well known from RTN studies, this is no longer the case for small-area devices, where only a handful of defects will contribute to the $\Delta V_{\rm th}$ shift. All these small-area devices will be essentially different. Thus, the distribution of the defect properties must be considered when device or circuit lifetimes are estimated. While it has been established a while ago that the number of defects in these devices follows a Poisson distribution [84], the fact that the capture and emission times of these defects are widely distributed was not appreciated until recently [27], [48], [85], [86]. Furthermore, the stochastic nature of charge trapping and emission will add to the variance [87]. Finally, due to the exponential distribution of the step heights in combination with the increased sensitivity of $\Delta V_{\rm th}$ to a *single* trapped charge (cf. Fig. 7), a single defect from the tail of the

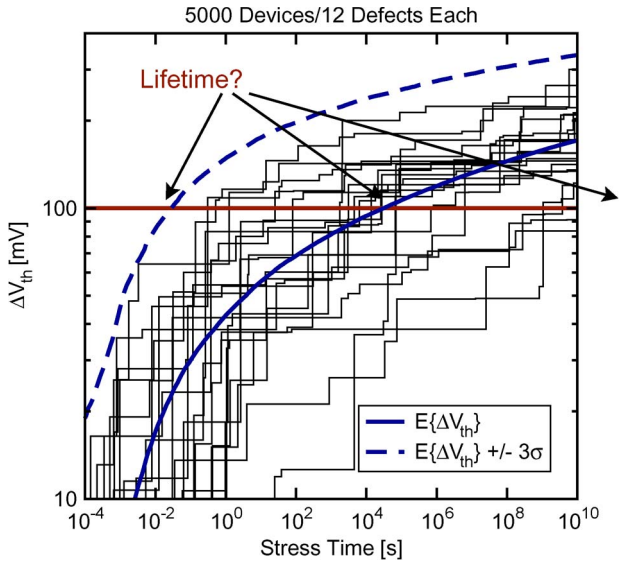

Fig. 22. In order to qualify a technology, degradation measurements have to be repeated on different devices (thin lines). Since each small-area device will have a different number of defects with different time constants, an estimate for the *lifetime can no longer be given* without detailed knowledge of the distribution of the time constants. This will *require a radical change in the qualification procedures*.

distribution may be sufficient to cause the failure of a device or circuit.

The significance of this effect is visualized in Fig. 21, where the simulated degradation of a device with 12 defects is shown. Even with fixed capture and emission times, as can be expected for a single selected device, repeated stress experiments will result in considerably different degradation curves. Thus, the lifetime can no longer be determined by monitoring the intersection of the degradation curve with a threshold value since each degradation curve will be different. As a consequence, the lifetime will show a considerable distribution. In practice, one is not that much interested in the degradation behavior of a single selected device but in the overall behavior of a technology. As such, since all devices will be different, the full distribution of the defect properties needs to be known [88]. Unfortunately, due to the wide distribution of the defect properties, the overall variance in the lifetime may become very large (see Fig. 22).

XI. Conclusion

We have summarized recent research activities leading to a paradigm shift in the understanding of NBTI away from the traditional RD theory toward a model based on switching oxide traps. The following features discussed in this paper may be worth highlighting:

1) NBTI recovery cannot be explained by the RD theory, irrespective of various claims in literature.
2) BTI up to at least 1 ks is *dominated by inelastic charge exchanges between preexisting defects and the substrate*.
3) RTN and the recoverable component of BTI are caused by the same defects, with *RTN* being their *quasi-equilibrium* and *BTI* their *nonequilibrium response*.
4) Charge trapping creates *switching oxide traps*. The charge state of these defects can follow the Fermi level in the substrate, thereby introducing a density of states into the silicon band gap. These switching traps explain the sensitivity of the recovery to positive biases.
5) Switching traps can contribute to both the threshold voltage shift and the charge-pumping current.
6) The precise microscopic nature of the defects causing BTI is still vague.
7) In *small-area devices*, the stochastic nature of charge exchange makes the *lifetime a stochastic variable*. Since every device will have a different distribution of defects, exact knowledge of the distribution of the time constants has to be acquired.

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