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Review paper

Controversial issues in negative bias temperature instability

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ABSTRACT

In spite of 50 years of history, there is still no consensus on the basic physics of Negative Bias Temperature Instability. Two competing models, Reaction-Diffusion and Defect-Centric, currently vie for dominance. The differences appear fundamental: one model holds that NBTI is a diffusion-limited process and the other holds that it is reaction-limited. Basic issues of disagreement are summarized and the main controversial aspects of each model are reviewed and contrasted.

1. Introduction

For > 50 years, NBTI (Negative Bias Temperature Instability) has been recognized as a fundamental reliability issue for metal–oxide–silicon (MOS) transistors. The last broad reviews of this topic were published in this journal over 10 years ago [1,2]. In the intervening years, the number of publications has surged with 5900 publications in the period 2006–2016 [3]. Fig. 1 shows the number of annual publications with the phrase “negative bias temperature instability” since 1990, illustrating a dramatic increase beginning around 2001.

In NBTI, positive charges build up in the MOS gate insulator due to the application of negative gate bias (V_g), exacerbated by temperature (T). Some of the positive charge may dissipate when V_g is reduced. NBTI became an important concern with the introduction of nitrogen in silicon oxynitride (SiON) gate dielectrics and continues to remain a crucial issue for high-k/metal-gate (HKMG) technology.

The new generation of NBTI specialists have significantly advanced the experimental and theoretical sophistication, yet no consensus has formed on the physical mechanism(s) governing the kinetics of NBTI during DC and AC stress and for recovery after stress, in large and small area devices. On the contrary, two disparate viewpoints have taken hold, typically referred to as the Reaction-Diffusion or “RD” model-based comprehensive framework [4] and the “Defect-Centric” model [5,6]. Simply put, one holds that NBTI is a diffusion-limited process and the other holds that it is reaction-limited. While oversimplified, this description illustrates the fundamental level of disagreement.

Historically, the RD model focused on the kinetics of interface trap (N_{it}) generation to explain NBTI degradation (the stress phase). In the early 2000s, researchers began to turn their attention to the relaxation phase, i.e., the recovery of the V_t shift when gate bias is removed, and the Defect-Centric model grew out of this emphasis. The RD model began as a continuum model while the Defect-Centric model was based on the discrete behavior of individual traps. This difference in approach has shaped much of the discussion, but ultimately both models aim to consistently explain both large-scale average behavior and microscopic behavior.

Broadly speaking, the *critiques* of these two models can be summarized thusly:

(1) While the RD model can now very successfully describe a large variety of observed data over a broad set of experimental conditions, the validity of the underlying physical interpretation is questioned [5] because the model parameters conflict with established literature on H in Si/SiO_2 systems;
(2) The Defect-Centric model has a strong basis in physics, supported by microscopic measurement of discrete defects, but until recently [7–9] it has paid scant attention to interface state generation, and the ability to comprehensively describe NBTI stress data over a broad set of process and stress conditions is questioned [10].

We give more details below and address these critiques. While both models have had good success in explaining experimental observations, neither model has achieved the sine qua non of theory by uniquely predicting an effect in advance of its observation, nor of achieving a consensus that the other model is inconsistent with experiment (in spite of several published attempts [5,10,11]).

This paper is not a comprehensive review of NBTI. In particular, we will not address material dependence in detail, such as different gate dielectrics or channel materials, nor statistical distributions, although such topics may eventually help to prove or disprove a model. Here, we

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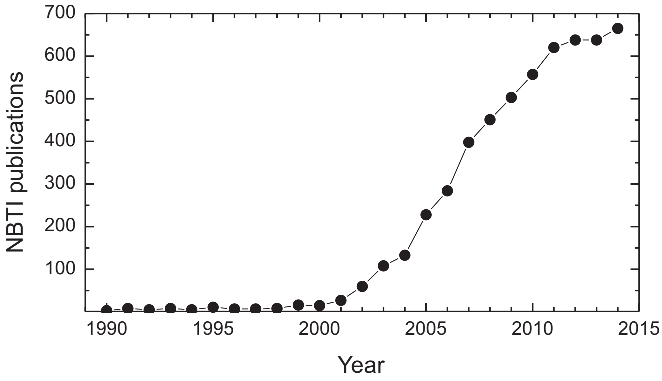

Fig. 1. Number of NBTI publications per year since 1990 [3].

outline the major controversies that continue to exist concerning the fundamental mechanisms.

2. Continuing controversies on basic issues

2.1. Roles of bulk traps and interface states

Experimental evidence shows that NBTI comprises both generated interface states (N_{it}) and hole trapping in bulk traps (N_{HT}, N_{OT}) [Reference [1] and references therein]. Interface states (N_{it}) are generally assumed to be responsible for changes in capacitance (CV), g_m degradation, and increased subthreshold swing as well as threshold voltage (V_t) shift when charged, and are frequently ascribed to the charge pumping (CP) or DCIV signals. Bulk traps can be either pre-existing hole traps (N_{HT}), or newly generated oxide traps (N_{OT}). They are often assumed to only affect V_t and give a rigid I_dV_g shift, although they can also contribute to DCIV and CP. However, there is still no consensus as to the most basic question of which component dominates the long-term V_t shift.

In the RD model, N_{it} generation – specifically, Si dangling bonds – dominates. Indeed, for state-of-the-art gate stacks, according to this model bulk trapping in pre-existing traps is insignificant, but new bulk traps can be generated under harsher stress conditions. The Defect-Centric model, on the other hand, focuses on hole capture and emission in bulk traps and border traps, which in this view dominate the process. Both models acknowledge that bulk traps can be generated under certain conditions, but the details of bulk trap generation are still being developed [7–9,12,13].

2.2. Interface state occupancy and recovery

During negative bias stress, interface states are not only created but they are positively charged; when the bias is removed, the occupancy changes and recovery (passivation) may happen [4,10]. The occupancy is important as only charged defects are sensed by measurement of V_t. The RD model includes an empirical interface state occupancy term with a stretched exponential spanning ~1μs to ~10s time constants, and passivation at longer times which is on the order of the stress time. Other researchers have claimed that neither component plays a significant role in normal recovery near zero bias [14]; occupancy changes of interface dangling bonds are too fast to be observed except by ultra-fast measurements, and passivation of interface states is either not observed at all, or only under certain conditions such as annealing at higher temperature.

2.3. Permanent vs recoverable components

Some of the early work on NBTI recovery decomposed NBTI into distinct recoverable (*R*) and permanent (*P*) parts [14]. This work claimed that *R* is due to hole de-trapping, and *P* is due to generated interface traps. To be more precise, it is now recognized that the "permanent" part is quasi-permanent on the time-scale of the experiments but can exhibit long-term recovery [15,16].

However, faster recovery has been reported in measurements like charge pumping, DCIV, and subthreshold slope, which are variously attributed to either N_{it} or oxide trap recovery [17,18]. In addition, the CP measurement itself accelerates recovery [16].

2.4. Measurement issues

Measuring NBTI turns out to be not straightforward, and no method exists which can measure NBTI directly and unambiguously without impacting the accumulated charges and defects and thus introducing some artifact. Therefore, most NBTI data leave some room for interpretation. In the following, the most commonly used measurement methods are discussed and their artifacts highlighted.

The conventional measure-stress-measurement (MSM) method first tries to establish a reference measurement, exposes the device to stress, and repeats the measurement to determine any changes. Typically, I_dV_g curves are measured to determine ΔV_t and Δg_m. However, as has been realized in the 2000s, I_dV_g measurements are inherently slow and the recovery occurring during that delay time leads to changes in the data.

In an attempt to minimize this delay, single-point measurements (sometimes called one point drop down) have been used which measure I_d only at a single gate voltage (typically near V_t) after a well-defined recovery/delay time t_{r0} rather than performing a complete I_dV_g sweep [19]. Conventional semiconductor parameter analyzers can perform this measurement in ~ms, and new instruments can perform it in ~10μs (so-called "*ultra-fast measurement*"). Different variants exist, e.g., measuring the shift in I_d at constant V_g, or the shift in V_g at constant I_d. In either case it is implicitly assumed that the major impact of NBTI is a rigid shift of the I_dV_g curve along the V_g axis and that the shape of the I_dV_g curve is only negligibly affected. This assumption may introduce some difficult-to-quantify errors for large degradation levels, although a final full I_dV_g can be used to estimate the impact.

In order to increase the amount of information, the recovery can be traced for a certain amount of time beyond t_{r0}, typically several decades, leading to what has been called the *extended MSM (eMSM)* method [20]. The impact of the measurement delay t_{r0} is clearly visible as the beginning of the recovery trace and only an extrapolation to $t_{r0} \rightarrow 0$ will give the true zero-delay degradation. This extrapolation requires some assumptions, in particular on the distribution of time constants. At the moment, it appears that it is impossible to measure fast enough to avoid this extrapolation as defects with time constants smaller than 1 μs exist which are difficult to measure.

In order to avoid this delay time problem, the *on-the-fly* (OTF) method was proposed which attempts to extract ΔV_t directly from the changes in the drain current I_d during stress [21]. Unfortunately, the on-the-fly method requires the measurement of a reference current $I_{d0} = I_d(t_{s0})$ at the start of stress, which has to be measured after a certain unavoidable minimum stress time t_{s0} which introduces an additional artifact [22–24]. In particular, t_{s0} has a strong impact on the power-law time exponent. Another drawback of the on-the-fly method is that I_d at stress voltage is more susceptible to changes in the mobility, which are difficult to separate from changes in the threshold voltage. In comparison, measurements done in the subthreshold regime depend exponentially on ΔV_t but only linearly on Δg_m, so most researchers no longer use the OTF method. In addition, OTF is not useful for measuring recovery.

Time-Dependent Defect Spectroscopy (TDDS) is a variant of eMSM, where repeated stress/recovery cycles on nanoscale devices are analyzed to build a 2D histogram of recovery step heights and times [25,26]. These steps occur with different heights, at stochastically distributed times, and the 2D histogram of recovery step heights and times reveals clusters corresponding to individual defects. TDDS provides the same information as eMSM, but additionally enables a statistical analysis of the steps heights and stochastically distributed times.

Although interface states are always present [27], in recent years researchers have mostly relied on simple V_t characterization, and ignore changes in g_m. In order to measure the number of interface states, other measurements are employed such as charge-pumping, CV, conductance, and DCIV. However, each of these have subtle issues when it comes to quantitative measurement, and their application can introduce other artifacts. For example, recovery is accelerated when the bias is switched towards depletion and accumulation [20,28].

A few important words of caution are necessary regarding the term “interface states”. Generally, everything that contributes to the charge pumping current or to DCIV is referred to as “interface states” and quite frequently it is assumed that these are P_b centers (silicon dangling bonds at the Si interface). While P_b centers are certainly the dominant interface states on unpassivated samples (without forming gas anneal), and also the dominant interface defect visible in electron-spin resonance measurements [27], it has been shown that P_b centers may not be the dominant contributors to ΔV_t and that other (non-ESR active) hydrogen related defects close to the interface are more important [20]. Only P_b-type defects have a plausible mechanism of passivation by hydrogen species, but they can likewise be de-passivated by atomic hydrogen; different species of defects will be *generated* rather than annealed by hydrogen reaction at the Si/SiO_2 interface [29]. In addition, ostensible bulk traps may also change occupancy based on Fermi-level position, giving rise to “slow” states or border traps which can also contribute to charge pumping and DCIV – especially in state-of-the-art ultrathin dielectrics where essentially all traps are border traps.

2.5. Different viewpoints

As mentioned in the Introduction, the developers of the RD model have emphasized the continuum, or average, behavior of V_t shift typical of large-area devices during the stress phase, using the above measurement techniques. The Defect-Centric groups focus attention on the microscopic behavior of individual traps using TDDS. Many of the critiques of each model can be attributed to this difference in approach, since all V_t-shift measurements require model assumptions in order to separate out various components: On the one hand, the RD model takes the 1/6 time-exponent for N_{it} as universal, since many recent ΔV_t data follow this dependence [30] and because it is consistent with the RD theory as well as with DCIV measurement – although the latter requires correction for the measurement delay and for the defect distribution in the band gap [10] in order to achieve quantitative agreement with the slope and magnitude of ΔV_t. This term is subtracted from the total V_t shift data in order to extract the other components, namely hole trapping (N_{HT}) and oxide trap generation (N_{OT}). This naturally leads to the conclusion that N_{it} dominates the degradation since total degradation trend is close to 1/6 time exponent. On the other hand, TDDS in nanoscale devices measures discrete de-trapping events, which are often ascribed to hole traps, and it is argued that interface traps give only a constant offset because they do not passivate during the time scale of the measurement and that changes in interface state occupancy are too fast to appear as steps in TDDS data, or in the recovery phase of eMSM [31].

3. Basics of the RD model

The basic physical mechanisms underlying the RD model have been confusing since they have been refined over time, so here we give a short description of the most recent understanding.

The RD model [4] presumes that inversion layer holes and oxide electric field assist in the breaking of H passivated defects at the Si/SiO_2 interface during stress, releasing H from Si—H bonds to form defects, presumed to be silicon dangling bonds (Si·), at the Si/SiO_2 interface. This is the *forward* reaction, schematically Si—H → Si· + H. Atomic H begins to accumulate in the Si/SiO_2 interfacial region until its concentration there becomes so large that the backward reaction (passivation of $Si^{\cdot}$) begins to balance the forward reaction, resulting in a quasi-equilibrium. This balance/equilibrium is assumed to be quickly established within about 1 s. In the next phase, this quasi-equilibrium begins to be slightly disturbed by hydrogen species diffusing away from this interfacial layer, leading to a gradual increase of Si dangling bonds with time, which follows a power law. This is the diffusion-limited regime, which dominates degradation for times larger than about 1 s according to the RD model.

The hydrogen species which diffuses is assumed to be H_2 which forms by defect assisted dimerization, i.e., reaction of released H with another H-passivated defect at the SiO_2/poly-Si interface, in the SiO_2 bulk, or for HKMG technology at the SiO_2/high-k interface or in high-k bulk; all bulk defects are lumped into an “effective interface” in the bulk for simplicity, referred to as the Double Interface Model [12]. This results in defect creation in the bulk (or internal interface) in addition to the Si/SiO_2 interface. Earlier versions of the RD model (now deprecated) assumed direct dimerization ($2H \rightarrow H_2$), or diffusion of atomic H rather than H_2.

In this model, interface state generation dominates NBTI and the fundamental assumption is that H or H_2 diffusion is slow and is the rate-limiting mechanism. H_2 diffusion gives $n = 1/6$ power-law time exponent [32] for long-time ($t > 1$ s) DC and AC stress, and the model predicts frequency independence for AC stress. H_2 diffusion is treated as non-dispersive; dispersive diffusion would result in T dependence of the power-law time exponent (n) of V_t shift [1]. This model has also been implemented in a stochastic version [33] in addition to the continuum version, resulting in identical prediction of N_{it} generation kinetics from the mean of multiple stochastic simulations.

The *backward* (recovery) process is then H_2 + Si· → SiH + H at the internal interface, followed by H + Si· → SiH at the first interface. During recovery diffusivity effectively slows in time, because during recovery H_2 has to hop and find dangling bonds at the internal interface, which becomes harder with the passage of recovery time as the unpassivated bond density reduces [4,34]. The diffusivity reduction involves one parameter, which has a fixed value which is different for planar devices and FinFETs [35]. In addition to interface state passivation, the V_t recovery transient includes a component due to the change of interface state occupancy (referred to as the *Transient Trap Occupancy Model* (TTOM)) which follows an empirical stretched exponential time dependence [4].

The RD theory is only used to describe interface state (N_{it}) generation and passivation. It must be supplemented with empirical stretched exponential models for hole trapping in pre-existing bulk traps (N_{HT}) to explain ultra-fast measured NBTI stress data, and for generation of new bulk gate insulator traps (N_{OT}) to explain stress data at high stress V_g and T conditions, and for transient trap occupancy [4]. All the 3 subcomponents (N_{it}, N_{HT} and N_{OT}) are assumed to be uncorrelated. From the result of examining numerous data sets, a picture has emerged where the N_{it} component is dominant at lower stress V_g and T, including at use condition, while the N_{OT} component becomes significant at higher V_g and T, and the N_{HT} component is mostly negligible in production quality devices across different technologies [4]. A maximum of 13 *process- or technology-dependent* parameters need to vary to explain the available stress and recovery data across different technologies, with all other model parameters fixed, and not all parameters need to be adjusted for process variation within a particular type of technology. These parameters comprise four parameters for the H-passivated bond dissociation process to create interface states at the Si interface (prefactor, activation energy, and two factors to model the field dependence and bond polarization); one adjustable parameter for the interface state occupancy term giving the fraction of generated interface states whose occupancy changes during a recovery process, plus the time constant and the stretched exponential parameter; three

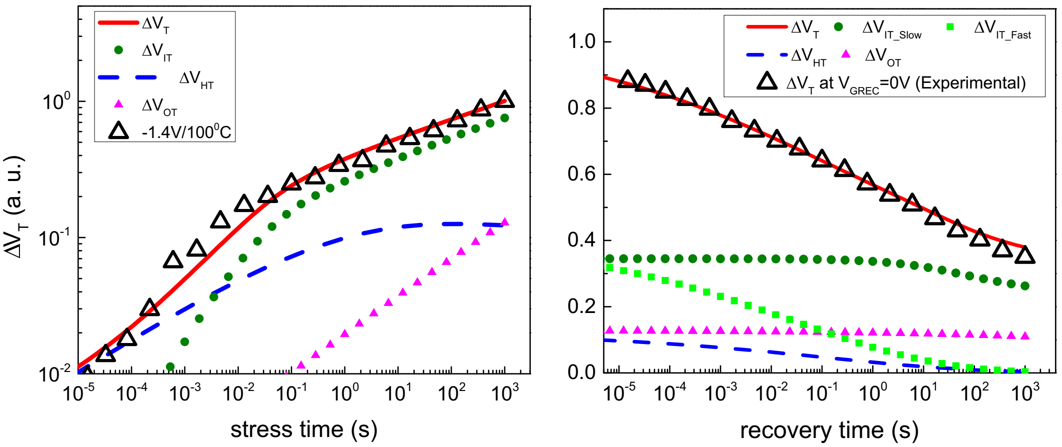

Fig. 2. NBTI component decomposition according the RD model. Data normalized to total ΔV_t at end of stress. Components are generated interface states (ΔV_{IT}), hole trapping in existing traps (ΔV_{HT}), and trapping in generated traps (ΔV_{OT}). Interface state recovery is further subdivided as passivation (ΔV_{IT_Slow}) and occupancy change (ΔV_{IT_Fast}). [Narendra Parihar, private communication].

adjustable parameters describing the N_{HT} term (density of traps, and two time constants for trapping and de-trapping); and one process-dependent pre-factor for bulk trap generation (N_{OT}). In addition, two constants for the number of available (passivated) bonds at the two interfaces (Si/SiO$_2$ and inside gate insulator bulk) will vary depending on surface orientation and oxide fabrication process. All other model parameters can be held to fixed values while describing a wide range of NBTI experimental data (DC and AC stress and recovery), across various types of devices (SiON, HKMG, different IL processes, Si and SiGe channels, planar, FDSOI, and FinFET). Each of these components is illustrated in Fig. 2.

4. Critique of the RD model

4.1. Unphysical parameterization of the RD model

In the RD model, it is assumed that the forward reaction Si—H → Si· + H is fast and is enhanced by the presence of holes in the channel as well as by the electric field because of the Si—H bond polarizability. However, this assumption is at odds with independent findings of hydrogen interaction with dangling bonds in Si/SiO$_2$. Both experimental data as well as DFT calculations indicate that the Si—H bond is extremely stable and should never break under BTI conditions. In particular, Si—H binding energies are in the range 2.5–3 eV, see Table I. Capture of a hole only marginally reduces this binding energy to about 2.3 eV. Also, the effective dipole moment of the positively charged Si—H bond is rather small, leading only to a small field dependence. Instead of direct dissociation, the conventional understanding is that Si—H bonds are broken and dangling bonds are created by reaction with atomic H released from elsewhere in the device, such as the substrate [36] or the gate [7–9], according to the exothermic [37] reaction Si—H + H → Si· + H$_2$.

Furthermore, the +/0 transition level of the Si—H bond is > 4 eV below the Si valence band making it very unlikely to capture a hole in the first place [38]. This is the reason for the effectiveness of dangling bond passivation by forming gas anneal, i.e., the energy level of the Si dangling bond is removed far from the Si bandgap by binding it with hydrogen. If Si—H could become easily charged it would show up as a threshold voltage shift, at least for high bias e.g., at readout above Vt or under stress condition. Overall, such large activation energies and deep energy levels make the Si—H bond extremely stable.

The RD model assumes a very small 0.2 eV barrier for the recovery process, H$_2$ + Si· → SiH + H. This is because in the double interface RD model the relative energy barrier between the forward and reverse processes of this reaction (or rather, the relative rate of the forward and reverse reaction, which also includes the pre-factors) must be approximately equal. Both forward and reverse barriers are taken as 0.2 eV, but this small value is only consistent with literature values for the *reverse* (dimerization) process. On the contrary, this recovery reaction – which is conventional forming-gas passivation – is effective only at temperatures above ~200C and reaction limited with measured activation energy of ~1.7 eV (See Table I).

Table I
Select RD model parameter values.

Reaction	RD model parameter	Literature value
SiH dissociation: energy barrier (SiH → Si· + H)	~0.5 eV (process dependent)	2.56 eV[a] 2.85 eV[b] 2.6 eV[c]
Si passivation by H$_2$: energy barrier (H$_2$ + Si· → SiH + H)	0.2 eV	1.7 eV[d]
H$_2$ diffusion coefficient at 125C	4×10^{-17} cm^2/s[e] 5×10^{-18} cm^2/s[f] 5×10^{-17} cm^2/s[g]	1.14×10^{-9} cm^2/s[h] 3.28×10^{-12} cm^2/s[i]

[a] K.L. Brower and S.M. Meyers, Phys. Rev. Lett. 72 (1990) 2745–2748.
[b] A. Stesmans, Phys. Rev. B 61 (2000) 8393–8403.
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[h] D. Griscom, J. Appl. Phys 58 (1985) 2524–2533.
[i] B.J. Fishbein, J.T. Watt, and J.D. Plummer, J. Electrochem. Soc. 134 (1987) 674–681.

In order for the RD model to agree with the shape of recovery data for long recovery time (as the number of unpassivated defects become small), a modification to the backward rate was introduced with an effective reduced diffusion rate at long time in recovery [4,12,34]. As described above, this was justified in terms of the added diffusion of hydrogen along the (mostly passivated) interface before encountering an unpassivated defect. However, critics can argue that it is unphysical to use different diffusion rates for stress and recovery. In the RD model the stress phase is characterized by a balance between the forward rate and the backward rate, so the same modification should be applied consistently.

Experimental evidence (Table I) suggests that H or H$_2$ diffusion in SiO$_2$ is very efficient and therefore not rate limiting. While the activation energies for diffusion used in the RD model are in the ballpark of the literature values, the pre-factors differ by about 5 to 8 orders of magnitude. To surmount the problem of H_2 diffusing too quickly through the insulator, in recent versions of the RD model diffusion is assumed to occur mostly in the poly-Si or elsewhere in the gate-stack.

Thus, while at a first glance the RD model appears to be based on previously established hydrogen chemistry, like breaking of Si—H bonds, annealing of dangling bonds in H or H_2, the diffusion of H and H_2, as well as dimerization of H to H_2, the parameters used in these reactions are at odds with extensive, well-established literature and industrial practice on hydrogen chemistry and interface state passivation processes, as shown in Table I.

4.2. Lack of microscopic evidence for hydrogen diffusion limited mechanism

If NBTI recovery is limited by the back-diffusion of hydrogen, the diffusion-limited nature requires the recovery time to roughly equal the stress time, simply because the hydrogen would have more time to diffuse away and thus needs more time to return to the interface to passivate the defect. In TDDS, the recovery steps would move to later times when the stress time is increased, but this has never been observed in TDDS. On the contrary, although new steps appear for longer stress times (so the average recovery time increases), those individual steps which were present for shorter stress time remain with the same mean emission time independent of stress time [11,39]. This experimental observation is perhaps the strongest evidence against diffusion in NBTI.

5. Response to Critique of the RD model

5.1. Parameterization

The experimental studies on Si—H bond energies cited in Table I are from electron spin resonance measurements, which detect only the P_b center and do not detect all interface defects [29]. The RD model only assumes that passivated defects are involved, and does not specify the defect. Furthermore, the energies are measured for the P_b center on the (111) interface. On the (100) interface, the P_{b0} center is the dominant paramagnetic center, and it has been shown that it is chemically different from the (111) defect [40].

The binding energy change due to hole capture was obtained using DFT calculations which are tricky for amorphous materials. On the other hand, the dependence of Si—H dissociation on electric field and hole density [41] is now being applied to describe trends with different Ge percentage in SiGe channel devices with a consistent set of model parameters [42–44].

The reported values of H_2 diffusivities have a large spread, and it reduces due to Nitrogen in the gate stack [45]. It might be speculated that high T is required for conventional forming gas annealing to bring H_2 to the Si/SiO_2 interface. For NBTI, H_2 is formed near the interface, and the reaction might proceed with small energy barrier for defects in the SiO_2 bulk, although there is currently no evidence to support this speculation.

5.2. Evidence for hydrogen diffusion limited mechanism

Hydrogen diffusion has been invoked since the very earliest days of NBTI [1], and the current state-of-the-art diffusion-based model provides a good description of ΔV_t kinetics during stress and recovery. The long-time power law time exponent of 1/6, which is broadly observed across devices (e.g., DCIV data corrected for delay time, and ΔV_t data under conditions where hole trapping is minimal) and circuits and across multiple technologies, is seen as verification of the diffusion process.

6. Basics of the Defect-Centric model

The defect-centric model [5] considers trapping and trap transformation through first-order processes, starting from the initial work by Huard et al. [14]. This group established that charge de-trapping was responsible for most of NBTI recovery and that interface states are much harder to anneal, and that recovery in small area devices proceeds in discrete steps, likely due to single hole de-trapping events.

The models invoked for trapping/de-trapping in defect-centric approaches have also been confusing as they have evolved over time in response to new experimental observations. We first briefly describe the current state-of-the-art model, followed by some simpler or earlier variants.

The most recent version (four-state switching trap model, a.k.a. multi-state model, or extended nonradiative multiphonon (NMP) model [5]) was inspired by the well-studied E' center (Si· in bulk SiO_2) which has metastable configurations in both the neutral state (the puckered version of the E' center), and also the positive state (the unpuckered variant) [46]. Thus, there are 4 states corresponding to neutral, charged and two metastable states. This model uses a detailed state-of-the-art physical chemistry model to describe the charge-transfer reactions [6]. The distribution of the rates follows from the distribution in the potential energy surfaces used to describe the state transitions. This model was introduced to explain observed differences in the bias dependence of capture and emission times in DC TDDS and RTN experiments, and also explains the subtle frequency dependence of NBTI seen in some experiments [47]. It is worth pointing out that the existence of a frequency dependence that goes beyond the simple first-order process is controversial, with some groups reporting frequency independent data.

During stress, the transition between neutral (1) and metastable (2′) states occurs via a multi-phonon process, and subsequently to a stable charged state (2) via a thermionic process. During recovery, the system traces back from (2) to (2′) to (1) for higher bias, and from (2) to (1) via another metastable state (1′) for lower bias. For the latter case, transition from (2) to (1′) occurs via a multi-phonon process and subsequently to (1) via a thermionic process. The full four-state model requires 11 physical parameters to describe a defect, but 9 of these can in principle be obtained from DFT calculations [48]. The only fitting parameters are then the trap position in the oxide and the capture cross section.

For most practical cases, e.g., measuring ΔV_t at a fixed readout voltage and fitting DC and AC stress/relax data at different duty cycles, the model can be condensed to an effective two-state model [49–51], which still uses a physical model for the charge-transfer reactions [6] and their dependence on energy levels and carrier concentrations. Distributions of both the trap position and cross section are needed to describe an ensemble of defects in a large area device.

In detailed physical models such as the four-state or two-state models just described, the first-order reaction rates follow from theoretical potential energy surfaces. The essential physics, however, is illustrated by the broadly distributed capture and emission times of each defect, in empirical *capture-emission time (CET) maps* [15], which are appropriate for a two-state defect (charged vs. uncharged, no metastable states) described by a first-order process. Equivalently, the distributions can be described by the effective activation energies for the forward and backward reactions [52], as illustrated in Fig. 3. The rates are empirically given by a bivariate normal distribution of forward and backward activation energies [15]. In this formulation, energy levels and carrier concentrations are lost and only the basic reaction-limited nature of the rates is preserved. This approach allows for a straightforward construction of CET maps which can be directly compared to experimental results, obtained from the second mixed derivative of V_t recovery curves, $\partial^2 V_t(t_s, t_r)/\partial \log(t_r)\partial log(t_s)$. In the CET map, the major difference between *R* and *P* is simply that both the capture and emission times of *R* are typically smaller than those of *P*. A CET map can be derived from any data set, either experimental or

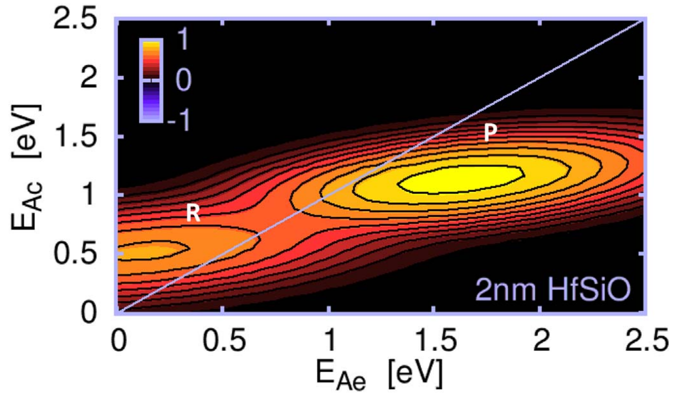

Fig. 3. Typical activation energy distributions (equivalent to CET map) for Recoverable (*R*) and quasi-permanent (*P*) components [15].

model-derived. For a first-order reaction model, the CET map corresponds directly to the defect density. For other models (e.g., RD) the corresponding CET map may not have a simple physical interpretation, but it would still be a complete mathematical description of the V_t time-dependence for a specific voltage and temperature condition. An empirical CET map can be constructed by assuming a distribution of capture and emission times (or distributed activation energies). As particularly important examples, if the energy distribution is assumed to be uniform the CET map model produces a log(t) time dependence. Gaussian and Fermi-derivative distributions give the experimentally observed t^n dependence [53].

An earlier Defect-Centric model [28], in a first attempt to explicitly account for separate *R* (charge trapping/de-trapping) and *P* (interface state) components, assumed that these components were coupled to maintain the structure of the previously-suggested triple-well model [54]. This coupling impacts the bias dependence of *P*. In later variants, which use a more accurate physical description of charge trapping, the components are uncorrelated, as they are in the current RD model. Thus, the quasi-permanent component (*P*) forms a second distribution in the CET map, as illustrated in Fig. 3.

In order to try to account for certain features of high temperature annealing or very long-term stress data (months), the role of atomic hydrogen release from the gate side has been proposed [7–9]. This model, as for the defect-centric approach generally, is reaction limited.

7. Critique of the Defect-Centric model

7.1. Lack of predictive capability for NBTI degradation under diverse stress conditions and materials

Critics claim [12] that most of the work involving defect-based models focuses on explaining the temporal kinetics of NBTI recovery after stress, and does not attempt to explain the temporal kinetics during DC and AC stress, especially long-time stress data. It is further argued [10] that the model has not been demonstrated to consistently explain both stress and recovery temporal kinetics after DC and AC stress over a broad range of conditions (bias, temperature, duty cycle and frequency) and across various types of devices (SiON, HKMG, different IL processes, Si and SiGe channels) and multiple data sets, using a consistent set of parameters, comparable to that shown by the RD model [4,10,30]. The four-state model has a large number of parameters related to multi-phonon and thermionic processes for the state transitions described above, which must be separately obtained for each material system. The analytic CET map models used in [15] are purely empirical and not directly linked to any microscopic physical model.

7.2. Ignores role of interface states

Critics argue [10] that NBTI recovery must be dominated by interface states because hole de-trapping is a relatively fast process with a time constant of ~0.1 s or less, and even the fast recovery component should include the neutralization of generated interface traps by electron capture, as previously illustrated in Fig. 2 above. Thus, ascribing fast recovery solely to hole de-trapping, and the long-term recovery of NBTI solely to a first-order process such as de-trapping, is argued to be conceptually wrong.

8. Response to Critique of the Defect model

8.1. Predictive capability

The time dependence during 10^4s stress and extrapolated to 10-year lifetime was shown using first-order kinetics based on empirical CET maps in [15], Fig. 14. Good agreement with recovery data after various stress times ranging from 2 s to > 10^4 s, and various voltages and temperatures, for SiO_2, SiON, and HK dielectrics, for DC and AC stress, has been demonstrated [28,55]. The defect-centric approach can also explain the improved NBTI in SiGe channel FETs due to the higher valence band, and CET maps obtained from simulations using the four-state model show good agreement with the broad characteristics of maps derived from experimenta data [56].

The CET maps of the reaction-limited picture successfully and naturally explain NBTI recovery temporal kinetics after AC stress (especially the delayed onset of recovery) via first-order reactions [6,15,52,57]. Depending on the stress/relax pattern, different regions of the CET map will be occupied, see Fig. 4. AC stress will result in a "missing corner" in the occupancy map, which is mostly composed of fast defects. As a consequence, recovery after AC stress will be much flatter but eventually merge with the DC recovery of the same effective stress time, as observed [55,57]. With changes in the duty factor α, the border of the triangular region in the CET map will be changed, explaining the duty-factor dependence [47,53,57].

The main driver of the defect-centric models, including the detailed four-state model, is to capture the correct, complex, physics. More work (in progress, e.g., [7–9,13]) is needed to uncover the physics of the creation of the quasi-permanent component. While the number of parameters in the full four-state model is large, they all have a well-defined physical meaning and may be taken for instance from DFT calculation, and are not merely empirical. However, not all of these details may be necessary for lifetime prediction, and a reduced model

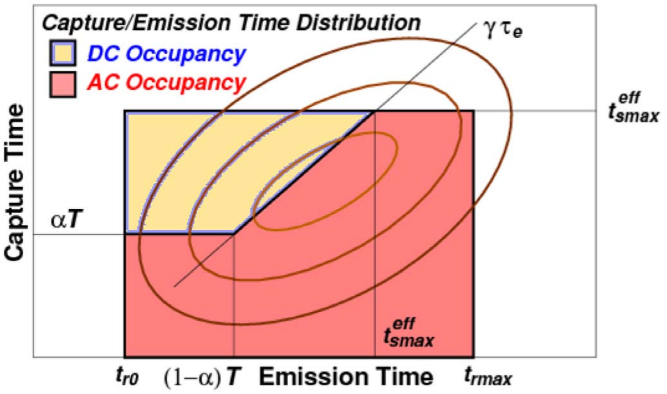

Fig. 4. Schematic occupancy in the CET map following AC (Duty factor-dependent) stress. After DC stress a rectangular region is addressed in the CET map. A more complicated shape results after AC stress, determined by the duty-factor α and the period T. The effective stress time is $t_{smax}^{eff} = \alpha t_s$, and $\gamma = \alpha/(1-\alpha)$ is the on/off ratio.

with a smaller number of parameters may serve the purpose well once the physics of the *P* component are better understood [49–51].

8.2. The role of interface states

Defect centric models have described the creation of both interface states and bulk traps using reaction-limited processes [14]. This unified treatment together with the CET nomenclature might lead to a misconception that defect centric models consider only charge trapping and ignore the creation of interface states. Interface states do contribute to CV, CP, and DCIV, but interface state occupancy changes do not contribute to TDDS data in the window 1 ms to 1ks. According to some interpretations of CP and DCIV data, the annealing of interface states is relatively slow unless accelerated by recombination events [15]. TDDS would therefore not see steps, but a constant offset to the ΔV_t trace due to newly created N_{it} [52]. Interface state occupancy changes follow SRH theory and would be too fast to be seen in TDDS or eMSM measurements. Furthermore, the capture time would only be weakly bias-dependent in inversion, in contradiction with experimental data. The focus is on bulk traps because they change their occupancy in the experimental time window.

9. Recommendations and Conclusions

Different approaches to the fundamental study of NBTI naturally lead to different conclusions, and so far, no consensus has emerged. Major differences of approach and assumptions are unresolved, and even such a basic issue as the time scale of interface state recovery is not agreed. In this paper, we have concentrated on the two major competing models. The large number of papers published on this topic (Fig. 1) contain many contradictory claims and have not led us any closer to consensus. The critical unresolved difference which appears unsurmountable at this time is that of diffusion-limited vs. reaction-limited processes, as this property remains the same no matter what modification is made to the basic scheme.

The criticisms of each model and the responses given in this paper are summarized below in the form of suggested actions to aid further development and improvements and to provide some benchmarks against which future publications can be evaluated.

R-D Models:

RD1. Demonstrate consistency of RD model with statistical properties of BTI degradation and recovery in nanoscale devices using TDDS data. Most prominent features to be captured are the distributions of the emission times as well as the variability of the step heights.
RD2. Provide independent physical confirmation for the parameters used, in particular the extremely low diffusion constants, the low barrier for Si—H breakage, the strong field dependence required for Si—H breakage, as well as the low barrier for the passivation of dangling bonds by H_2.
RD3. Provide a physical model for the stretched exponential time dependence of the occupancy of interface states (TTOM) and demonstrate consistency with D_{it} measurements (e.g., CP, DCIV, or CV data).
RD4. Confirm the validity of the time-dependent effective diffusion constant used for recovery, e.g., by stochastic modeling.

Defect-Centric Models:

DC1. Demonstrate quantitative prediction of NBTI V_t shift (short- and long-time kinetics of stress and recovery; voltage and temperature dependence) using physics-based models (not empirical CET maps) for DC and AC stress with various duty factors and frequencies.
DC2. Provide a quantitative prediction of interface traps in stress and recovery in large area devices using a physics-based model and demonstrate consistency with Dit measurements (e.g., CP, DCIV, or CV data).
DC3. Provide the decomposition of stress and recovery into components (interface states, trapping/de-trapping, etc.) and their individual dependence on voltage, temperature, etc.
DC4. Provide physical description of process dependence of NBTI kinetics using consistent model parameters for (a) low and high N in gate stack, (b) different Ge percentage in channel (c) Si capped SiGe devices for different Si cap, and (d) FinFET vs bulk planar devices.

By focusing attention on these specific areas, we expect that various aspects of each model could eventually be validated, resulting in a hybrid model which retains elements of each. For example, the oxide trap generation component in the RD model formulation, which is currently empirical, could incorporate the defect-centric model trapping picture. However, it is important to emphasize that both models cannot continue to be promulgated independently and without further proof of their validity. Merely demonstrating the ability to fit data does not constitute such proof. Scientific theories do not become more valid by doing “more of the same” experiments, or fitting the same model to multiple data sets. It is imperative for researchers to focus on the experimental observations that are clearly incompatible with current theories.

Some aspects of common understanding may already begin to emerge. For example, most researchers agree on a role for hole trapping and de-trapping with a distribution of time constants, even as they disagree on its importance in describing the net threshold voltage shift. Similarly, researchers agree on the importance of newly created defects, although their relative contribution during stress and recovery at use conditions remains controversial [58], and most agree that hydrogen reactions with defects must play some role, even if the details are quite disparate. Ultimately, the stretched exponentials, distributions of diffusion constants, and dispersive reaction-limited processes seen in the current models may converge to a single picture.

In contrast to the attempt to understand NBTI at the microscopic level, most microelectronics researchers today take a pragmatic, empirical approach to estimating long-term NBTI degradation and the impact of fabrication process changes. It would certainly be preferable, though, to have a predictive, physically-sound model which allows simulation under diverse circuit operation conditions. Several attempts in this direction have been published [59–62], but without a consensus these models remain speculative.

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