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Critical analysis of short-term negative bias temperature instability measurements: Explaining the effect of time-zero delay for on-the-fly measurements

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Recently several groups have used the reaction-diffusion (R-D) model with H₂ diffusion in interpreting negative bias temperature instability (NBTI) degradation. While the classical “H₂ R-D” model can interpret long-term NBTI behavior, it is inconsistent with short-term stress data obtained by recently developed ultrafast measurements and widely used on-the-fly measurements. Moreover, experimental data from various techniques are not consistent with each other. Here, the authors show that the H₂ R-D model must be generalized to consistently interpret NBTI at all time scales. The generalized model highlights the previously unappreciated role of time-zero delay in reconciling differences among the so-called delay-free on-the-fly measurements. © 2007 American Institute of Physics. [DOI: 10.1063/1.2695998]

Negative bias temperature instability (NBTI), a major degradation mechanism for *p*-type metal-oxide-semiconductor devices biased in inversion, results in variation of transistor parameters and is generally monitored through threshold voltage shift (ΔV_T). The origin of such degradation has been debated for the last few years, and it is now generally accepted that, for devices with SiO₂, plasma SiON, and thin thermal SiON gate dielectrics, NBTI degradation results mainly from depassivation of Si-H bonds at the Si/dielectric interface and resultant diffusion of hydrogen species into gate dielectric and poly-Si.¹⁻⁸ As such, several groups have used the reaction-diffusion (R-D) model to interpret NBTI degradation.¹⁻⁷ At long stress time ($t_{\text{stress}} > 10\text{--}100$ s), ΔV_T shows a power law behavior when plotted with respect to time ($\Delta V_T \sim At^n$) with a consistent time exponent (n) of $\sim 1/6$. This time exponent is independent of the measurement techniques used to monitor ΔV_T [e.g., ultrafast measurement (UFM),⁹ “delay-free” on-the-fly I_{dlin} measurement (OTFM),^{2,3,5,6,8} etc.]. The R-D model attributes the robust (constant over several decades in time⁴) long-term $n \sim 1/6$ exponent to the diffusion of molecular hydrogen (H₂).^{3,7} This “H₂ R-D” model also provides a consistent interpretation of temperature and field dependencies of NBTI for long-term stress, as extensively studied for devices with SiO₂, plasma SiON, and thin thermal SiON dielectrics.^{2,5,6,8}

Although the classical “H₂ R-D” model provides an excellent interpretation for long-term stress data, our analysis shows that (1) the predictions of this model is *inconsistent* with the short term, sub- 10 s, NBTI degradation [see Fig. 1(b)] and (2) in contrast to long-term degradation, the short-term time exponent of NBTI degradation depends on the measurement techniques. In this letter, we show that the inconsistency between theory (“H₂ R-D” model) and experiment arises from the implicit assumption in the “H₂ R-D” model that atomic to molecular hydrogen (H to H₂) transformation is instantaneous. Once this assumption is relaxed and the model is generalized to explicitly account for both H and

H₂ (“H-H₂ R-D” model), one can consistently interpret NBTI data at all stress times (Fig. 1). We also trace the differences in short-term time exponents obtained using various techniques to the previously unappreciated role of time-zero delay for OTFM. Once the time-zero delay is accounted for, the “H-H₂ R-D” model explains experimental data at all time scales independent of measurement techniques (Fig. 2).

As stated earlier, *long-term* NBTI stress can be explained with the “H₂ R-D” model as shown in Fig. 1(b). This figure also signifies that H₂ diffusion (alone) cannot properly explain the short-term stress data with the parameters normally used in the model.^{2,3,5-7} Whereas H₂ diffusive model

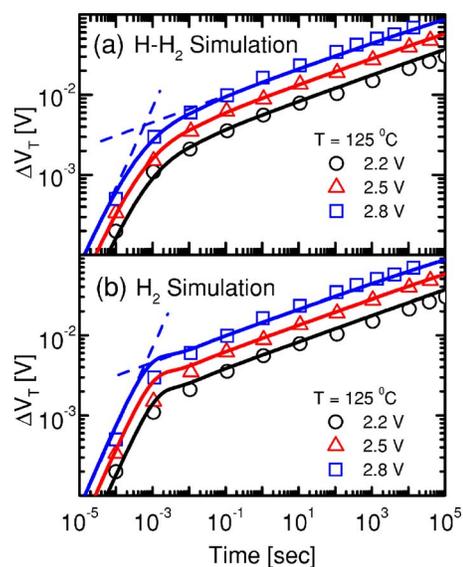


FIG. 1. (Color online) (a) Generalized R-D model (H-H₂ system) can explain the experimental trends (Ref. 9) at any stress time. R-D model parameters [consistent with literature (Refs. 3, 6, and 19)]: $k_f = 6 \times 10^{-3} E_c \exp(0.65 E_{ox}) \text{ s}^{-1}$ [E_c : oxide electric field due to mobile carriers; E_{ox} : total oxide electric field], $N_0 = 5 \times 10^{12} \text{ cm}^{-2}$, $k_r = 3 \times 10^{-9} \text{ cm}^3 \text{ s}^{-1}$, $D_H = 3 \times 10^{-13} \text{ cm}^2 \text{ s}^{-1}$, $D_{H_2} = 1.8126 \times 10^{-14} \text{ cm}^2 \text{ s}^{-1}$, $k_{H_2} = 1.4 \times 10^{-3} \text{ cm}^3 \text{ s}^{-1}$, $k_{H_2} = 95.4 \text{ s}^{-1}$. (b) Classical H₂ R-D model (with large k_H and k_{H_2}) cannot explain short t_{stress} data consistently. The dashed asymptotes in (a) and (b) indicate that the transition from reaction to H₂ diffusion for H-H₂ system is slower compared to a classical H₂ system.

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predicts a change in n from 1 (for reaction-limited region^{1,7}) to 1/6 (for H₂ diffusion-limited region^{3,7}) within approximately one order of time scale (see the dashed asymptotes in Fig. 1(b)), experiments indicate a wider transition region (Fig. 1), approximately three to four orders of magnitude.

The inability of the “H₂ R-D” model to explain the short-term stress condition indicates that the assumption of instantaneous formation of H₂ immediately after the dissociation of Si–H bond (creating interface traps), while appropriate for analysis of long-term degradation, may not be appropriate to interpret short-term data. This requires explicit consideration of H within the R-D framework, as this should be the first by-product after interface trap generation, before getting transformed to H₂.^{3,7} Although neutral charge state may not be a stable form of atomic hydrogen, its transient formation is indeed possible.¹⁰ Therefore, in the generalized R-D model, diffusion of both H and H₂ and H ↔ H₂ conversion are explicitly incorporated in the R-D framework by the following equations:¹¹

$$\frac{dN_{\text{IT}}}{dt} = k_f(N_0 - N_{\text{IT}}) - k_r N_{\text{IT}} N_{\text{H}}^{(0)}, \quad (1)$$

$$\frac{dN_{\text{H}}}{dt} = D_{\text{H}} \frac{d^2 N_{\text{H}}}{dx^2} - k_{\text{H}} N_{\text{H}}^2 + k_{\text{H}_2} N_{\text{H}_2}, \quad (2)$$

$$\frac{dN_{\text{H}_2}}{dt} = D_{\text{H}_2} \frac{d^2 N_{\text{H}_2}}{dx^2} + \frac{1}{2} k_{\text{H}} N_{\text{H}}^2 - \frac{1}{2} k_{\text{H}_2} N_{\text{H}_2}. \quad (3)$$

In Eq. (1), k_f , k_r , N_0 , N_{IT} , $N_{\text{H}}^{(0)}$ are defined as^{1-3,11} the Si–H bond-breaking rate, Si–H bond-annealing rate, initial bond density available before stress, interface trap density, and hydrogen density at the Si/dielectric interface, respectively. In Eqs. (2) and (3), k_{H} and k_{H_2} represent the generation and dissociation rates of H₂; D_{H} and D_{H_2} represent the diffusion coefficients for H and H₂; N_{H} and N_{H_2} represent the concentrations of atomic and molecular hydrogen.¹¹ Equations (1)–(3) reduce to the classical “H₂ R-D” model [Eq. (3) of Krishnan *et al.*³] if k_{H} and k_{H_2} are so large that H ↔ H₂ transformation becomes instantaneous.

Our simulation results, based on the solution of Eqs. (1)–(3), show that the dominance of H ↔ H₂ conversion during short-term stress extends the transition between reaction-limited region ($n \sim 1$) and H₂ diffusion-limited region ($n \sim 1/6$) by several orders of time scale, enabling excellent fit for short-term NBTI degradation [see Fig. 1(a)]. Later when H ↔ H₂ conversion reaches quasiequilibrium, H₂ diffusion dominates and results in $n \sim 1/6$. We use the extensively verified field dependence of k_f (Ref. 6) to interpret the voltage-dependent data in Fig. 1. This figure also shows that the generalized “H–H₂ R-D” model *at long times* predicts the same time exponent as the “H₂-only R-D” model, because in steady state, diffusion of H₂ governs the dynamics of interface trap generation.¹² Slightly lower n , observed for experimental long t_{stress} data in Fig. 1(a), can be attributed to the decrease in (stress) electric field as a function of time. NBTI causes $|V_T|$ to increase, hence for a constant stress bias, the oxide electric field decreases. Our numerical calculation predicts a decrease in n to ~ 0.15 [typically observed for OTFM (Refs. 2, 5, and 8)] for maximum stress condition of Fig. 1(a). Moreover, as similar stress field dependence of k_f explains NBTI stress data at all stress times in Fig. 1(a),

we recognize that for these devices, *any contributions to ΔV_T from hole trapping is negligible*. Further, since activation energies for hole trapping,⁹ H and H₂ diffusion, and N_{IT} generation^{2,3,6,13} (represented by $E_{A(\text{HT})}$, $E_{A(\text{H})}$, $E_{A(\text{H}_2)}$, $E_{A(\text{IT})}$, respectively) are such that $E_{A(\text{HT})} \ll E_{A(\text{H})} < E_{A(\text{H}_2)} \sim E_{A(\text{IT})}/n$, models involving hole trapping⁹ would be inconsistent with temperature-dependent data for these specific experiments.

Next we address the puzzle of measurement-dependent n values for *short-time* degradation (see Fig. 2). Extracting the physics behind NBTI degradation at any stress time requires one to obtain the exact nature of ΔV_T using some experimental setup. Indeed classical I_D - V_G measurement provides an incorrect estimate of n at mid- to long stress time, due to unintentional recovery inherent in the measurement technique.^{2,14} The uninterrupted OTFM eliminates the “recovery” problem^{2,5,8,14-16} and calculates ΔV_T by: (a) $\Delta V_T(t) = |(I_{\text{dlin}}(t) - I_{\text{dlin}}(t_0))/I_{\text{dlin}}(t_0)| * V_{GTO}$ (Refs. 2, 5, 8, and 14) (see Ref. 17 for details about the calculation done by Rangan *et al.*¹⁴), (b) $\Delta V_T(t) = \int_{t_0}^t \partial I_{d,\text{sense}} / g_{m,\text{sense}}$,¹⁶ or (c) $\Delta V_T(t) = M |(I_{\text{dlin}}(t) - I_{\text{dlin}}(t_0))/I_{\text{dlin}}(t_0)|$.¹⁵ These methods give comparable results for long-term NBTI stress.¹⁵ A point that is not always obvious, hence ignored, is the use of t_0 in the above calculation. Exact ΔV_T measurement using OTFM mandates the use of $t_0 = 0$. Yet OTFM setups require some time (≥ 1 ms) before measuring $I_{\text{dlin}}(t_0)$; as a result $t_0 \neq 0$ (termed as time-zero delay) in such measurements. Therefore, while solving the issue of unintentional recovery at each measurement step, OTFM introduces an error in degradation estimates due to nonzero t_0 , the effect of which will be particularly important at short stress times. Such t_0 error is not present either in classical I_D - V_G measurement (which is erroneous due to recovery issue, discussed earlier) or in the UFM, because in these cases $\Delta V_T(0)$ is obtained *before* the device is stressed. To observe the effect of time-zero delay in the OTFM results, we have used the experimental data from Reisinger *et al.*⁹ (at $V_{G,\text{stress}} = -2.2$ V, 125 °C), with a specified measurement delay of ~ 1 μs (hence very small recovery) and $t_0 \sim 0$ (similar to classical I_D - V_G), as reference. Once correction due to t_0 is accounted for, we can explain n

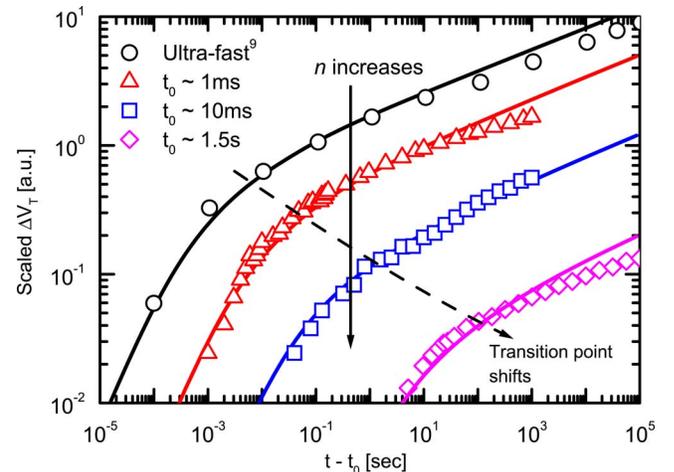


FIG. 2. (Color online) Effect of t_0 on OTFM compared with UFM, for similar stress conditions. Here, $\Delta V_T(t-t_0) \sim |(N_{\text{IT}}(t) - N_{\text{IT}}(t_0))/N_{\text{IT}}(t_0)|$ and data are scaled along the Y axis for clarity. As t_0 is increased, there is an increase in time exponent at a particular $(t-t_0)$ mainly in the short-term stress and also a rightward shift of the apparent transition point when the system reaches steady state with H₂ diffusion.

for all OTFM data in Fig. 2, having various $t_0 \neq 0$. The figure indicates that the use of $t_0 \neq 0$ in calculating $\Delta V_T(t)$ for OTFM results in an “apparent and artificial” increase of n mainly in short-term NBTI degradation. Indeed, if t_0 is very high (>1 s), even the longer-term stress data may be effected by t_0 delay. This delay explains the discrepancy of OTFM results from different experimental groups^{2,14,18} regarding the onset of the $n \sim 1/6$ regime (see Fig. 2). As consideration of t_0 delay alone can explain the variation of n in Fig. 2, any possible contribution from hole trapping must have fully saturated⁹ before t_0 and hence will have no effect in plotted ΔV_T . Therefore, when devices have comparatively few hole trapping,⁸ our results imply that once the t_0 delay is corrected for, the OTFM results would be consistent with each other and predict the same degradation as the UFM method. And these t_0 -corrected experimental data can then be interpreted by the H–H₂ model [Fig. 1(a)]. As a practical matter, if such t_0 correction of OTFM is difficult, our simulation suggests that reasonable projection for NBTI lifetime can still be made if t_0 is kept below 0.2 ms and projection is based on the data above 1 s. On the other hand if hole trapping is significant (as would be the case for films having thick thermal SiON dielectric⁸) and saturates before t_0 , time-zero delay correction allows one to extract back *only* the component of the degradation due to interface traps. To determine whether hole trapping had saturated before t_0 in high $N_{\text{interface}}$ samples, one should make a second calculation/measurement with higher time-zero delay and check whether the same ΔV_T vs t (for $t_0=0$) can be simultaneously extracted back from both data sets.

In conclusion, we have illustrated how a generalized H–H₂ R-D model can consistently explain the NBTI degradation at both short- and long-term stresses. We trace the previous discrepancy between theory and measurements to the assumption of “instantaneous H₂ formation” in the classical model. Further, we demonstrate that the existing discrepancy in short-term NBTI data by various measurement techniques can be attributed to contamination by time-zero delay in OTFM systems. Our analysis suggests that lifetime prediction^{4,6} and projection back to operating condition⁶ must be carried out using long-term NBTI stress data (having $n \sim 1/6$), obtained after $t_{\text{stress}} \sim 100$ s with $t_0 \leq 1$ ms, because

higher exponents in short-term degradation can result in unnecessarily pessimistic projections.

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