

NBTI: AN ATOMIC-SCALE DEFECT PERSPECTIVE

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Abstract-- We utilize a combination of MOSFET- gate controlled diode DC-IV measurements and a very sensitive electrically-detected electron spin resonance technique called spin-dependent recombination to observe and identify defect centers generated during NBTI in fully processed SiO₂ and plasma nitrided oxide (PNO)-based pMOSFETs. In SiO₂ devices, we observe the NBTI-induced generation of two Si/SiO₂ interface silicon dangling bond centers (P_{b0} and P_{b1}) and very likely an oxide silicon dangling bond center (E'). Our observations indicate that both P_{b0} and P_{b1} defects play major roles in these SiO₂-based devices and also suggest that E' centers could play an important role. In PNO devices, we observed the NBTI-induced generation of a new defect center which is fundamentally different from the P_{b0}/P_{b1} defects generated during NBTI in SiO₂ devices. Our results indicate that it plays a dominating role in NBTI-induced interface state generation in thin PNO devices and also exhibits a post-negative bias temperature stress (NBTS) recovery. Although we observe different interface state defects, we observed essentially equivalent activation energies in both the SiO₂ and PNO devices. [Keywords: negative bias temperature instability, interface traps, MOSFET, spin-dependent recombination]

I. INTRODUCTION

NBTI is a major reliability concern for modern CMOS technology. It causes a shift in threshold voltage (V_t) and a degradation in saturation drain current (I_{d,sat}) [1-2]. Until recently, NBTI has been a relatively small reliability obstacle; however, aggressive gate oxide scaling coupled with less aggressive scaling of operating voltages and the incorporation of nitrogen in the gate oxide has exacerbated the problem [1-2]. NBTI electrical measurements [1-6] analyzed in terms of a reaction-diffusion model has lead to a widely held hypothesis that NBTI arises from interface state generation by the depassivation of hydrogen atoms at a Si₃≡SiH site at the Si/SiO₂ interface. The exact details of this degradation process are still controversial [5], particularly the atomic-scale mechanisms that change the NBTI response in nitrided oxides. However, there is only very limited direct experimental evidence regarding the atomic scale nature of the NBTI process.

Electron spin resonance (ESR) is essentially the only tool with the analytical power and sensitivity to observe atomic-scale defects associated with MOS instabilities such as NBTI. ESR has proven useful in monitoring atomic scale defects that play important roles in many CMOS reliability problems [7]. In a pioneering study, Fujieda *et al.* successfully utilized conventional ESR measurements to study NBTI interface state generation [8-10]. Their experiments, however, involved large area (~1 cm²) bare oxide structures on p-type substrates. It would be much more preferable to make measurements on fully processed devices. Spin dependent recombination (SDR) is a highly sensitive electrically detected ESR technique which enables

measurements on fully processed, technologically relevant, transistors [11]. In this study, we employ SDR to directly observe the atomic scale defects associated with NBTI in fully processed SiO₂ and PNO devices. We observe that NBTS generates (P_{b0}/P_{b1}) interface state defects and probably an oxide silicon dangling bond defect (E') in thicker SiO₂-based devices. Fujieda *et al.* had previously noted the generation of P_{b0}/P_{b1} centers. P_{b0} and P_{b1} defects are both silicon dangling bond defects in which the central silicon atom is back-bonded to three other silicon atoms at the Si/SiO₂ boundary. The main differences between the two defects are in the dangling bond axis of symmetry [12-13] and in differences in the defects' electronic density of states [14-18]. However, in contrast to the reports of Fujieda *et al.* [8-10], we observed that NBTS generates a completely new defect center in PNO-based devices. Despite this fundamental atomic-scale difference in defect generation, the defect generation activation energies for both PNO and SiO₂ devices were found to be equivalent within experimental error.

II. EXPERIMENTAL METHODS

Interface state densities (D_{it}) were monitored using DC-IV gate controlled diode measurements [19-20] on large area (~40,000 μm²) pMOSFETs with source and drain contacts shorted together. In the gate controlled diode DC-IV measurement, the source and drain are shorted, the source/drain to substrate diode is slightly forward biased (0.33V in our measurements), and the source/drain to substrate recombination current is measured as function of gate bias [19-20]. Fitzgerald and Grove [19] found that the change in recombination current ΔI_{sub} (difference between the peak and the baseline) scales with the interface state density; and can be approximated by

$$\Delta I_{SUB} = \frac{1}{2} q n_i \sigma_s v_{th} D_{it} A q |V_F| \exp\left(\frac{q|V_F|}{2kT}\right) \quad (1)$$

where q is the electronic charge, n_i is the intrinsic number of carriers, σ_s is the geometric mean of the electron and hole capture cross section, v_{th} is the thermal velocity, A is the effective gate lateral area, V_f is the forward bias applied to the source/drain to substrate junction, k is the Boltzmann's constant, and T is the temperature. The change in recombination current (ΔI_{sub}) is proportional to the interface state density within an energy window ½ q|V_f| [19].

Activation energies were extracted using the uninterrupted stress technique with -50 mV on the drain electrode [6]. The measurements utilized 1x10 μm² pMOSFETs and monitored the percentage degradation in I_{d,lin} after 6000 seconds of NBTS.

Room-temperature SDR measurements were made on the same devices utilized in DC-IV measurements and were carried out at X-band (microwave frequency ~ 9.5 GHz) with two custom-built SDR

spectrometers (one based on a Resonance Instruments 8330 series microwave bridge the other on a Bruker ER380 Series ESR spectrometer with variable temperature control to allow for in-situ NBTS and SDR). All magnetic resonance measurements were made in a TE₁₀₂ microwave cavity and were calibrated using either a strong pitch spin standard and measurement of microwave frequency or measurement of both microwave frequency and magnetic field using an EIP 535 frequency counter and Resonance Instruments 515 nuclear magnetic resonance gaussmeter respectively.

A brief, only qualitatively correct, explanation of SDR provided by Lepine [21] may be useful in understanding our results. Lepine's model combines both the Shockley-Read-Hall (SRH) model for recombination and the Pauli exclusion principle. A SRH recombination event occurs when a conduction electron is captured by a deep level defect and then a hole is captured at the same defect site. (The recombination sequence could also be reversed.) In SDR, a transistor is placed in a large slowly varying DC magnetic field that partially aligns the spins of the conduction electrons, the holes, and the deep level defects. If a deep level defect and a charge carrier have the same spin orientation, the Pauli exclusion principle forbids charge capture by the deep level defect because the electrons must have different spin quantum numbers to occupy the same orbital. When a paramagnetic deep level's electron spin resonance condition is satisfied, the defect's electron spins are "flipped." Flipping the spins increases the probability of opposite spin orientations between deep level defects and charge carriers, thus increasing the recombination current. This increase in recombination current is what is measured in SDR.

Lepine's model provides simple insight into the physics governing SDR but predicts a spin dependent change in the recombination current of approximately 1 part in 10⁶ at the fields and temperatures utilized in our study [21]. SDR experiments can show a current change of approximately 1 part in 10⁴ or larger [22]. A more accurate (but more complex) description of SDR has been proposed by Kaplan, Solomon, and Mott (KSM) [23]. The KSM model extends Lepine's model to coupling of two spins prior to the actual recombination events. The KSM analysis is more nearly consistent with experimental data than the Lepine model [22]. The details of these SDR models and their relevance to MOS devices are discussed elsewhere [22].

III. RESULTS

A. 75Å SiO₂ Devices

Figure 1 shows the pre- and post-NBTS DC-IV characteristic curves for 75Å SiO₂-based devices subject to -5.7V at 200°C for 20,000 seconds. The NBTS generates a large increase in the peak recombination current which is proportional to the interface state density. Following the analysis of Fitzgerald and Grove [19] and assuming a capture cross-section $\sigma = 1.4 \times 10^{-16} \text{ cm}^2$, we extract an NBTI-induced D_{it} (pre-stress $8.2 \times 10^9 \text{ cm}^{-2}\text{eV}^{-1}$, post-stress $1.6 \times 10^{12} \text{ cm}^{-2}\text{eV}^{-1}$). Figure 2 illustrates the corresponding SDR measurement. The increase in D_{it} is accompanied by the generation of both P_{b0} ($g = 2.0060 \pm 0.0003$) and P_{b1} ($g = 2.0033 \pm 0.0003$) interface states as well as the generation of a third defect that we likely attribute to an E'_v center oxide defect ($g = 2.0007 \pm 0.0003$). The g -value is most simply defined as $g = h\nu/\beta H$, where h is Planck's constant, ν is the microwave frequency, β is the Bohr magneton, and H is the magnetic field [7]. The P_{b0} and P_{b1} defects have been shown to be the dominating interface defects in Si/SiO₂ systems [7].

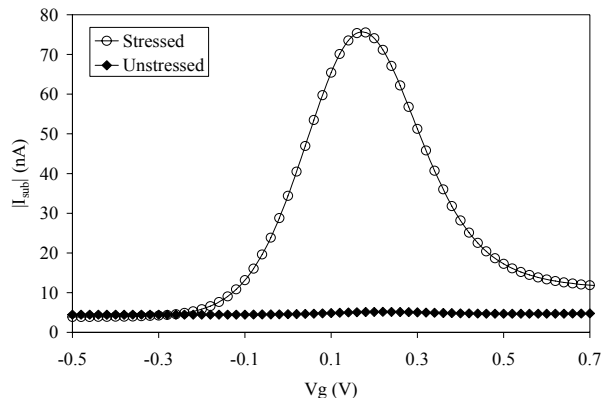


FIGURE 1. DC-IV MEASUREMENTS OF 75Å SiO₂ pMOSFET BEFORE AND AFTER THE APPLICATION OF NBTS (-5.7V AT 200°C FOR 20,000 SECONDS) INDICATING THAT THE NBTS GENERATES A LARGE INCREASE IN D_{it} . (SOURCE/DRAIN TO SUBSTRATE VOLTAGE = 0.33V)

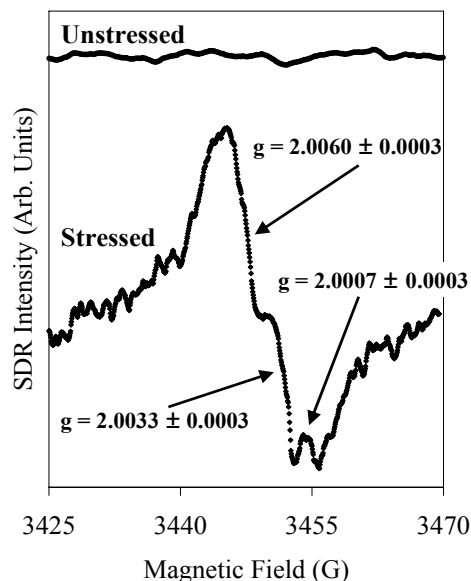


FIGURE 2. SDR TRACES OF 75Å SiO₂ pMOSFET BEFORE AND AFTER THE APPLICATION OF NBTS (-5.7V AT 200°C FOR 20,000 SECONDS) INDICATING THAT THE NBTS GENERATES P_{b0}/P_{b1} INTERFACE DEFECTS AS WELL AS THE LIKELY GENERATION OF AN E'_v OXIDE DEFECT CENTER.

B. 23Å PNO Devices

Figure 3 shows the pre- and post-NBTS DC-IV characteristic curves for 23Å EOT PNO devices subject to -2.8V at 145°C for 15,000 seconds. It is again clear that the NBTS generates a substantial increase in D_{it} . We were unable to extract precise values for D_{it} because the capture cross section of the trapping defect centers in these PNO devices is not yet known; however, the NBTS generated an increase in ΔI_{sub} of slightly more than an order of magnitude, which suggests about an order of magnitude increase in D_{it} . Figure 4 illustrates the corresponding SDR measurement on this PNO device. The increase in D_{it} is accompanied by the generation of a new defect with zero-crossing $g = 2.0020 \pm 0.0003$, as well as the generation of, as yet poorly resolved, side peaks approximately $\pm 26\text{G}$ from the center

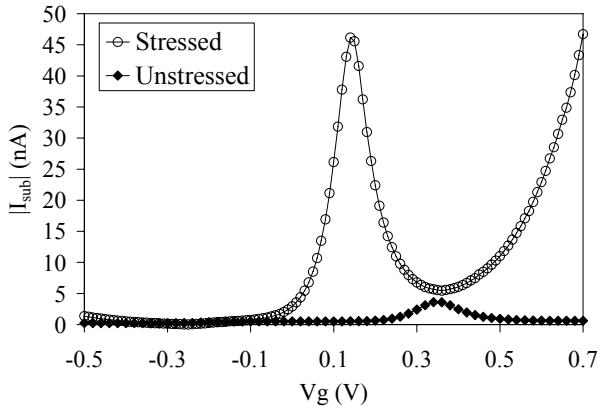


FIGURE 3. DC-IV MEASUREMENTS OF 23Å PNO pMOSFET BEFORE AND AFTER THE APPLICATION OF NBTS (-2.8V AT 145°C FOR 15,000 SECONDS) INDICATING THAT THE NBTS GENERATES A LARGE INCREASE IN D_{it} . (SOURCE/DRAIN TO SUBSTRATE VOLTAGE = 0.33V).

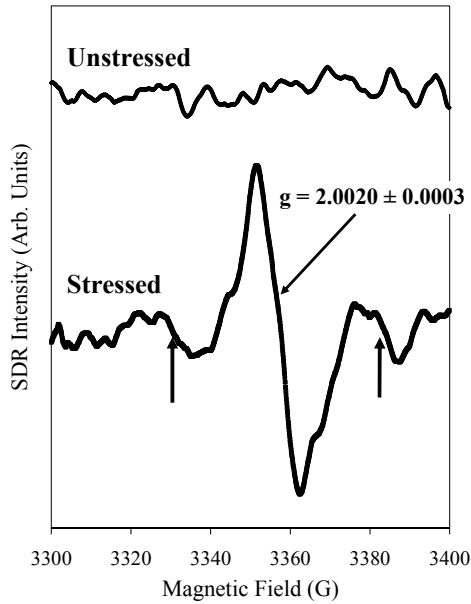


FIGURE 4. SDR TRACES OF 23Å PNO pMOSFET BEFORE AND AFTER THE APPLICATION OF NBTS (-2.8V AT 145°C FOR 15,000 SECONDS) INDICATING THE GENERATION OF A NEW INTERFACE STATE DEFECT CENTER AT $g = 2.0020$ AS WELL AS THE GENERATION OF SIDE-PEAKS.

signal. The center signal has a g -value that would be consistent with a silicon dangling bond in which the central silicon atom is back-bonded to oxygen atoms (an E' -like defect) [24-26]. The side peaks indicate the presence of defects that involve electrons coupled to magnetic nuclei, in this case, almost certainly nitrogen and/or hydrogen. (The side peaks also indicate that more than one defect is present.) We are not yet able to identify the dominating center signal with certainty, but can state, with certainty, that the NBTS-induced interface defect in the PNO devices is fundamentally different than the defects observed in the SiO_2 devices. Figure 5 illustrates this difference in g -value by comparing the (a) 75Å SiO_2 devices and the (b) 23Å PNO devices with virtually identical spectrometer settings (With these spectrometer settings, the P_{b0} , P_{b1} , and E' defect

signatures in the SiO_2 devices are artificially broadened so as to overlap.) The difference in observed g -values is well beyond experimental error and is a direct indication that we are observing different interface defects in the PNO devices.

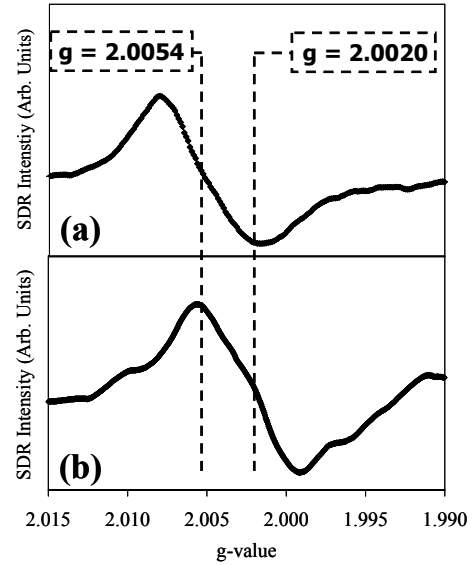


FIGURE 5. SDR TRACES OF (A) 75Å SiO_2 ($g = 2.0054$) AND (B) 23Å PNO ($g = 2.0020$) pMOSFETs ILLUSTRATING THAT THE INTERFACE STATE DEFECTS GENERATED IN THE SiO_2 ARE FUNDAMENTALLY DIFFERENT THAN THOSE GENERATED IN THE PNO DEVICES. NOTE : SPECTROMETER SETTINGS ARE SUCH THAT THE USUALLY OBSERVED P_{b0}/P_{b1} DEFECT SIGNATURES IN SiO_2 OVERLAP.

C. 23Å PNO Recovery

In an effort to further investigate the nature of this new NBTS-induced interface defect, we employed in-situ DC-IV and SDR measurements to observe NBTI recovery [27]. Figure 6 illustrates DC-IV characteristic curves taken pre- and post-NBTS (-2.8V 140°C for 10,000 seconds) as well as during the recovery process. The

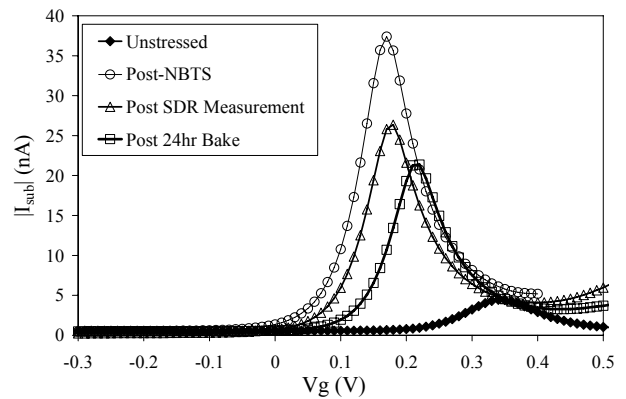


FIGURE 6. DC-IV MEASUREMENTS OF 23Å PNO pMOSFET PRE- AND POST-NBTS (-2.8V AT 140°C FOR 10,000 SECONDS) AS WELL AS POST-SDR MEASUREMENT AND POST-24HR BAKE (150°C WITH 0V ON THE GATE ELECTRODE). THIS INDICATES THAT D_{it} EXHIBITS A RECOVERY PROCESS POST NBTS. (SOURCE/DRAIN TO SUBSTRATE VOLTAGE = 0.33V)

NBTS generates a large increase in D_{it} (approximately an order of magnitude). A subsequent DC-IV measurement after ~ 5 hours of SDR measurement shows a reduction in D_{it} associated with recovery. After both DC-IV and SDR measurements, the device was subject to a 24-hour bake (150°C with 0V on the gate electrode). A DC-IV measurement post-bake shows only a modest amount of recovery. We believe that the lack of post-bake recovery is due to the temperature quench post-NBTS required for room temperature SDR measurements. Thus, the NBTS stress is “locked-in” when cooling to room temperature and is relatively unaffected by additional high temperature treatments [6]. Figure 7 illustrates the corresponding SDR measurements taken at various post-NBTS time-steps. NBTS, again, generates a signal at $g = 2.0020 \pm 0.0003$ and the amplitude of that signal (which is proportional to the number of defects) degrades during recovery. Figure 8 summarizes the D_{it} and SDR signal intensity decrease during the recovery processes. Since the observed signal at $g = 2.0020 \pm 0.0003$ shows a recovery behavior that qualitatively scales with the observed D_{it} degradation, these results are a strong indication that this defect plays a major NBTI role in PNO devices.

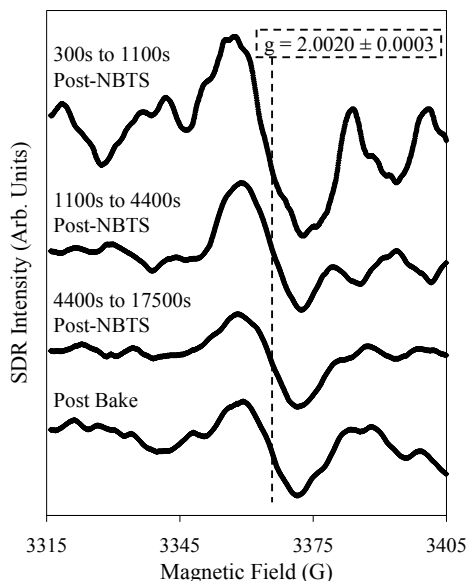


FIGURE 7. SDR TRACES OF 23\AA PNO pMOSFET POST-NBTS (-2.8V AT 140°C FOR $10,000$ SECONDS) AT VARIOUS TIME STEPS WHICH SHOWS THAT THE DENSITY OF THE NEWLY OBSERVED SIGNAL AT $g = 2.0020$ ALSO EXHIBITS NBTI RECOVERY. (SIGNAL SIZE SCALES WITH THE DENSITY OF DEFECTS.)

D. 27\AA SiO_2 and 23\AA PNO Activation Energy

Figure 9 illustrates an Arrhenius plot of both 27\AA SiO_2 and 23\AA PNO devices. The extracted NBTI activation energies are observed to be time-independent and are essentially equivalent ($0.11\text{--}0.12$ eV).

This result is contrary to reports that show that the activation energy is different for SiO_2 and PNO devices [28-29]. It is consistent with the idea that the rate limiting step involves the diffusion of species to and/or from the atomic defects. This result is therefore consistent with the recent work of Alam [2] *et al.* as well as the very recent work of Varghese [30] *et al.* who have proposed that the activation energies for SiO_2 and PNO devices should be equivalent because the activation energy is essentially determined by the diffusing species. Regardless of the observed fundamental difference between interface

defects in SiO_2 and PNO devices, our observations strongly suggest that the diffusing (presumably hydrogenic) species are the same in both SiO_2 and PNO devices.

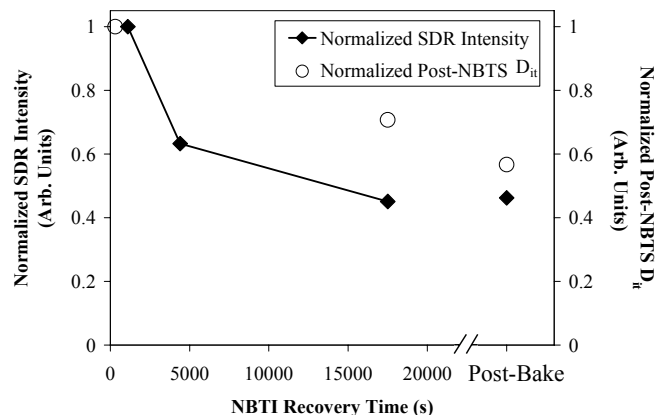


FIGURE 8. NORMALIZED SDR SIGNAL AMPLITUDE AND NORMALIZED POST-NBTS D_{it} AS A FUNCTION OF NBTI RECOVERY TIME ILLUSTRATING THE NBTI RECOVERY PROCESS QUALITATIVELY TRACKS WITH THE DENSITY OF THE NEWLY OBSERVED DEFECT.

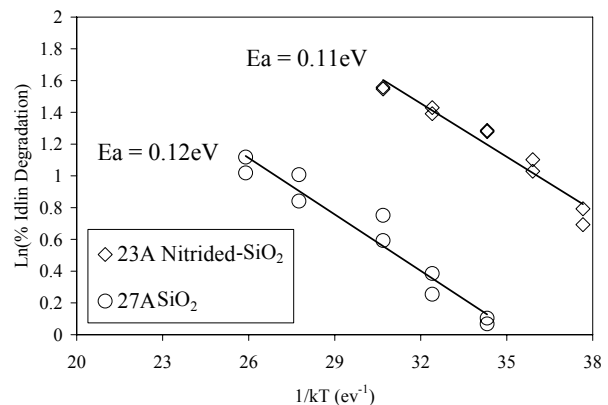


FIGURE 9. ARRHENIUS PLOT FOR SiO_2 AND PNO pMOSFETs STRESSED AT -3.3V FOR 6000 SECONDS. ACTIVATION ENERGIES ARE EXTRACTED BY MONITORING THE DEGRADATION IN I_{DLIN} USING THE UNINTERRUPTED STRESS METHODOLOGY. BOTH DEVICES ARE FOUND TO HAVE ESSENTIALLY THE SAME ACTIVATION ENERGIES.

IV. DISCUSSION

The observation of P_{b0} and P_{b1} defects as the NBTI-induced defects in thicker SiO_2 -based devices is generally consistent with many studies of the electronic response of pMOSFETs to NBTS in that the P_{b0} and P_{b1} defects both exhibit densities of states that are consistent with NBTI damage. The P_{b0} has a broadly peaked density of states with the “+ / 0” and “0 / -” transitions separated by about 0.7eV and centered approximately about mid-gap [14-16]. The P_{b1} has a narrower density of states with the “+ / 0” and “0 / -” transitions separated by $\sim 0.2\text{--}0.3\text{eV}$ and shifted toward the lower part of the gap [18]. For pMOSFETs biased in inversion, both the P_{b0} and P_{b1} centers would be positively charged and would result in the correct

NBTI-induced shift in threshold voltage. At this time we are unable to determine the exact role of E'_γ defects in thicker SiO_2 devices. Considering the NBTS condition (-5.7V, 200°C for 20,000 seconds), we cannot rule out the possibility that, under these circumstances, the E'_γ centers have been generated via hot hole oxide injection [31]. However, a number of NBTI models invoke cracking of H_2 as a result of the presence of a hole in the oxide [2]. There is clear experimental evidence that E'_γ centers can capture holes and that this hole capture event allows the defect to crack molecular hydrogen [26]. Thus a role for E' centers may be generally consistent with many NBTI investigations.

The observation of a central signal at $g = 2.0020 \pm 0.0003$ in thinner PNO devices is consistent with the presence of a member of the E' family [24-26]. The E' family of defects involves electrons primarily residing in one or more silicon orbitals in which the silicons are back bonded to oxygens [24-26]. Many E' variants have been discussed in the literature (E'_α , E'_β , E'_γ , and E'_δ) [24, 25]. Two frequently observed MOS E' variants, the E'_γ and the E'_δ or EP defects, involve a silicon dangling bond or bonds in which the silicon is back bonded to three oxygen atoms or an oxygen vacancy site [26]. The E'_δ defect has a zero-crossing g-value ($g = 2.0019$) which is very similar to our observations while the E'_γ defect has a zero-crossing g-value (2.0005) [26]. The E'_δ defect is believed to be an oxide hole trap in which the positive trapped charge and the unpaired electron are equally shared between two silicon atoms on either side of the vacancy [32]. The more commonly observed E'_γ can be caused by a hole trapped in an oxygen vacancy [7]. However the same E'_γ ESR line shape is also generated by an electrically neutral single silicon dangling bond [26]. Earlier studies of relatively thick oxides have shown that both E'_γ and E'_δ defect centers tend to be localized near the Si/ SiO_2 boundary [26]. The (oxygen vacancy variant) E'_γ defects have also been shown to act as efficient switching traps and, when close enough to the Si/dielectric boundary, can also act as recombination centers [7, 33, 34]. Despite the very plausible link between the newly observed NBTS-induced defect in PNO devices and E' centers, the identification should be regarded as somewhat tentative. This is so for several reasons. First, the SDR signal-to-noise is fairly modest; it is certainly good enough to rule out any possibility that the defect signal is caused by a P_{b0}/P_{b1} center but it is not good enough to definitively assign the spectrum to E' centers. Secondly, the link between E' centers and NBTI may (or may not) be difficult to reconcile with the observation that whereas E' densities are generally enhanced by very high temperature annealing [7], the NBTI response is greatly improved by such anneals [35]. The conflicting high temperature anneal response might be a result of the fact that these E' centers are confined within an ultrathin dielectric region.

Fujieda *et al.* reported that the addition of nitrogen in the gate dielectric caused a modification to the P_{b1} structure that lowered the g-value ($g = 2.0027$) for the magnetic field orientated parallel to the Si/dielectric normal [9-10]. Recall that the g is actually a second rank tensor quantity. If we were observing such a modified P_{b1} structure, the center's g-value would depend upon sample orientation in the magnetic field. Upon 90 degree rotation of the device (100) surface normal with respect to the magnetic field we observe, within experimental error, no change in g-value (not shown). This strongly suggests that although the observed defect is located very nearly at the interface, the defect's presence extends slightly beyond the silicon into the amorphous dielectric. (This would be consistent with a tentative link to the E' family.)

The absence of P_{b0}/P_{b1} signals in the stressed PNO devices suggests that the structure of the unstressed Si/dielectric interface is

different in ways that are important to device reliability. It is quite likely that the P_{b0}/P_{b1} center precursors are silicon dangling bonds at the interface which have been passivated by hydrogen. The density of the P_{b0}/P_{b1} center precursors is almost certainly determined by the mismatch between SiO_2 bonding and Si bonding. The P_{b0}/P_{b1} precursor sites likely act to relieve interface strain. Typically, the near interface SiO_2 is in compression. If this compressive strain were somehow to be reduced in the PNO processing (which likely introduces nitrogen to the near Si/dielectric region) the density of P_{b0}/P_{b1} center precursors would be reduced. The introduction of oxide oxygen vacancies (likely the E' center precursors) would also tend to reduce the strain in the near Si/dielectric interface region.

It may be that the presence of far fewer P_{b0}/P_{b1} centers is the direct result of an increased presence of E' centers and/or nitrogen atoms- both seem likely to reduce interfacial strain.

IV. CONCLUSIONS

We observe NBTI-induced atomic-scale defects in SiO_2 and PNO devices. In fairly thick SiO_2 devices, P_{b0} and P_{b1} interface defect centers play dominating roles in D_{it} generation while the E'_γ centers could play somewhat different role. In thinner PNO devices, we observe a new defect with a zero-crossing g-value of $g = 2.0020 \pm 0.0003$. This defect appears to play a dominating NBTI role in the PNO devices and is fundamentally different than what is observed in SiO_2 based devices. The new defect exhibits NBTI-recovery that qualitatively scales with D_{it} . Despite these fundamental differences in SiO_2 and PNO interface defects, we measure activation energies that appear to be the same. This strongly suggests that the rate limiting step is diffusion and that the, presumably hydrogenic, diffusing species is the same in both SiO_2 and PNO devices.

V. ACKNOWLEDGMENTS

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