APPLIED PHYSICS LETTERS **96**, 223509 (2010)

Observations of negative bias temperature instability defect generation via on the fly electron spin resonance

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(Received 22 December 2009; accepted 19 April 2010; published online 4 June 2010)

We demonstrate "on the fly" electron spin resonance (ESR) in which the defect generation process in the negative bias temperature instability (NBTI) can be observed without recovery contamination. Elevated temperature and modest negative gate bias generates ESR spectra due to E′ center defects. The NBTI generated E′ center spectrum disappears upon stress condition removal, a result consistent with recovery. Our observations support the idea that NBTI is triggered by inversion layer hole capture at an E′ precursor site which leads to depassivation of nearby interface trap precursors. © *2010 American Institute of Physics*. [doi:10.1063/1.3428783]

The negative bias temperature instability (NBTI) is the most important reliability problem facing microelectronics technology.[1–4] It occurs when p-channel metal-oxide-silicon (MOS) field-effect-transistors are subjected to negative gate bias at elevated temperature; resulting in a threshold voltage shift and degradation of saturation drive current. [4] A fundamental understanding of the physical processes involved in NBTI has yet to be established.[1–3]

NBTI has been explained in terms of a reaction-diffusion model in which inversion layer hole capture during NBTI stress leads to hydrogen liberation from passivated interface states.[1–3] The liberated hydrogenic species diffuses into the gate oxide leaving behind an unpassivated interface state; in pure SiO_2 gate devices, the interface state defects are P_b centers.[5–7] In the reaction-diffusion model, recovery is explained as the reversal of this process; when the NBTI stress is removed, the hydrogenic species diffuses back to the Si/SiO_2 interface and repassivates the interface states.[1–3] Although the reaction-diffusion model generally makes physical sense, many variations exist and none fully explain the entire NBTI response, particularly recovery.[1] A universally accepted model explaining NBTI is not available.

Conventional electron spin resonance (ESR) observations of Fujieda *et al.*[5] on blanket capacitor structures and recent electrically detected magnetic resonance (EDMR) observations of Campbell *et al.*[6–8] on fully processed transistors show that NBTI is dominated by Si/SiO_2 interface traps called P_b centers in pure Si/SiO_2 gate dielectric devices. Campbell *et al.*[6–8] also reported EDMR detection of E′ center generation under heavy NBTI stressing conditions. (P_b centers are Si/SiO_2 interface silicon dangling bond centers).[9]

Campbell *et al.*[7,8] and Lenahan[10] have proposed that the NBTI process might be triggered by the capture of (silicon inversion layer) holes, which simple statistical mechanics arguments indicate[10] would lead to subsequent P_b center generation via loss of hydrogen at P_b-H precursor sites. (The hole capture process can create a positively charged E′ site in which one side is a neutral singly occupied silicon dangling bond and the other a positively charged diamagnetic silicon). These arguments linking E′ hole capture and P_b generation have been detailed elsewhere in the context of NBTI (Ref. 11) and earlier in the context of radiation damage.[12–14] Extensive experimental evidence for E′ and P_b hydrogen interactions has also been reported.[12–14] E′ defect charge exchange with the silicon valence band has also been documented by Conley *et al.*[15,16] in earlier studies in the context of radiation damage.

Recently, Grasser *et al.*[17] developed a comprehensive quantitative two stage model for NBTI. In this model, NBTI is also triggered by inversion layer hole capture at an E′ center precursor site (a neutral oxygen vacancy). The presence of the oxide silicon dangling bond created in this process (the neutral side of the E′ center) then triggers the creation of poorly recoverable defects (P_b centers) via an E′/P_b center hydrogen exchange. The comprehensive quantitative model of Grasser *et al.*[17] greatly expands upon the earlier more qualitative arguments[7,8,10] and explains NBTI degradation over a wide range of bias voltage and stress temperature, the observed asymmetry between stress and recovery, and the strong sensitivity to bias and temperature during recovery. Central to the model is the prediction that paramagnetic E′ centers will be present during stress, and will, for the most part, very quickly recover upon removal of stress.

As mentioned previously, Campbell *et al.*[6–8] reported only somewhat tenuous E′ experimental observations in NBTI stressed devices. The tenuous nature of these observations is likely due to two reasons. First, the EDMR technique of spin dependent recombination (SDR) utilized by Campbell *et al.* does not permit observations at significant negative gate bias. To obtain reasonable SDR sensitivity, the stress biasing conditions must be altered so that the electron and hole quasi-Fermi levels are split more or less symmetrically about the intrinsic Fermi level at the Si/SiO_2 interface.[9,18] If the theory of Grasser *et al.* is correct, this would invariably lead to significant recovery of the E′ centers; in the Campbell *et al.* measurements, most of the E′ centers would be electrically neutralized and thus no longer paramagnetic. Second, even under optimized biasing conditions, SDR is only marginally adequate for E′ center detection because E′ centers are less effective recombination centers than Si/SiO_2 P_b centers; only those E′ centers close to the interface contribute to SDR.[18] However, conventional

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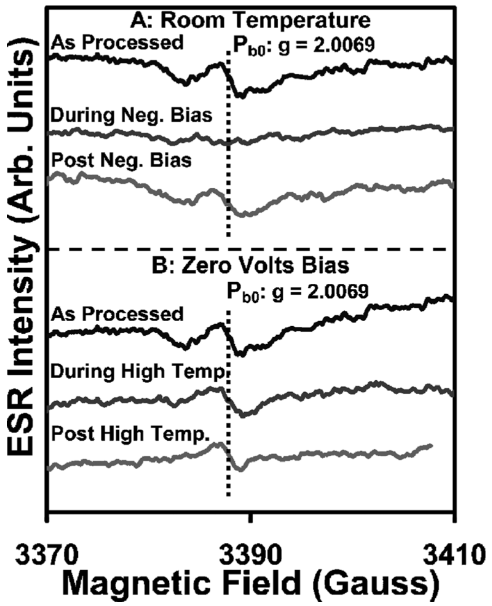

FIG. 1. (a) Room temperature ESR traces taken on the sample as-processed (top), with −25 V bias (middle), and after removal of negative bias (bottom). (b) Three ESR traces for the sample as-processed (top), with 0 V bias at 100 °C (middle), and after cooling the sample back to room temperature (bottom). Negative bias alone [Fig. 1(a)] or the elevated temperature alone [Fig. 1(b)] does not generate additional P_b interface states or E′ defects within the resolution of the measurement. Prestress P_{b0} defect densities are about 8×10^{10} cm^{-2} in each case.

ESR permits E′ center detection at any gate bias, provided the E′ center is paramagnetic.[9] The E′ center oxygen vacancy would be paramagnetic when positively charged. We have developed an on the fly approach in which ESR measurements are performed during negative bias stressing of MOS structures at elevated temperature. In this approach, ESR measurements are made while the device structure is under negative bias stress at elevated temperature, which, unlike prior ESR studies, allows for the observation of NBTI defects void of any recovery contamination.

The samples used in this study are large area Si/SiO_2 blanket capacitor structures with 49.5 nm thermally grown SiO_2 oxides which were treated with a postoxidation forming gas anneal. ESR measurements were performed before, during, and after the sample was subjected to a modest NBTI stress of −25 V (oxide field <5 MV/cm) at 100 °C. Negative bias was applied to the sample utilizing corona ions to provide a virtual gate.[19] The gate bias was monitored before and after stress with a Kelvin probe. The thick (49.5 nm) oxides were chosen to ensure a constant gate bias over the measurement time (several hours). A suprasil "cold finger" apparatus was modified to heat the sample inside the microwave resonant cavity. ESR measurements taken at negative bias and at room temperature [Fig. 1(a)] indicate that the negative oxide bias alone does not create any additional interface states or oxide defects within the measurement resolution. ESR measurements taken at elevated temperature and zero oxide bias [Fig. 1(b)] indicate that elevated temperature alone does not create any additional interface states or oxide defects either. ESR measurements were made on a Bruker Instruments X-band spectrometer with a TE_{104} microwave cavity and were calibrated with a weak pitch standard. Spin densities are accurate to about a factor of 2 in absolute number.

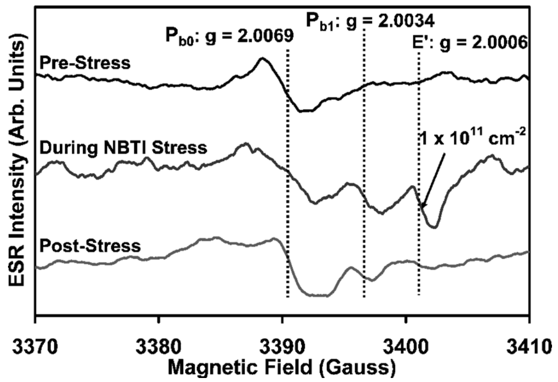

FIG. 2. Three ESR traces on the sample before stress (top), during NBTI stress (middle) and after stress (bottom). Note the clear generation of an E′ signal during NBTI stress (middle), as well as P_{b1} center generation, and the nearly complete recovery of the E′ defects poststress (bottom). Note that, due to differences in spin lattice relaxation times, the amplitude of the P_b signal is disproportionally large compared to the E′ signal.

Figure 1(a) illustrates three ESR traces all taken at room temperature. The top trace was taken on the as-processed sample, the middle trace was taken with the sample biased with −25 V (bias maintained for several hours during measurement), and the bottom trace taken after removing the negative bias. The as-processed sample displays a weak signal consistent with a P_{b0} Si/SiO_2 interface state ($g=2.0069$). (The g is 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 at resonance. The g depends on the defect's structure and its orientation with respect to the applied magnetic field).[20] The room temperature corona bias of −25 V (middle) does not create any additional interface states (P_b centers) or oxide defects (E′ centers). It does suppress the P_{b0} signal because these defects are interface traps and can respond to the substrate silicon Fermi level. (The negative bias renders most P_{b0} centers positive and ESR inactive). Figure 1(b) illustrates three ESR traces all taken at 0 V bias. The top trace was taken on the as-processed sample at room temperature, the middle trace was taken with the sample at elevated temperature (100 °C), and the bottom trace taken after returning the sample to room temperature. The elevated temperature at 0 V bias (middle) does not result in an increase in interface states or oxide defects.

Figure 2 illustrates three ESR traces taken on the sample before, during and after NBTI stress. Each trace was signal averaged for several hours. Although these measurements are slow, recovery is nonexistent since the stress conditions remain constant throughout the measurement. The spectrometer settings used were chosen to permit the observation of both Si/SiO_2 P_b centers and SiO_2 E′ centers and are not optimized for either defect; the E′ center density is under-represented in these traces. (A significant difference in E′ and P_b spin lattice relaxation times lead to this under-representation).[19] In the prestress case (top), we observe a weak single line spectrum with $g=2.0069$ which is due to P_{b0} Si/SiO_2 interface states. During NBTI stress (middle), we observe the clear generation of Si/SiO_2 P_{b1} centers ($g=2.0034$) and SiO_2 E′ centers ($g=2.0006$). Upon removal of the stress, the $g=2.0006$ E′ center signal completely recovers while some of the P_{b1} centers remain. This result clearly indicates that positively charged oxygen va-

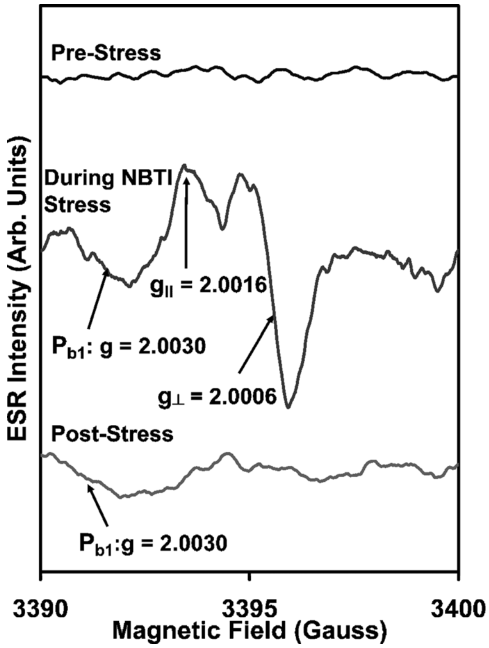

FIG. 3. Three ESR traces taken on the sample before stress (top), during NBTI stress (middle) and after stress (bottom). In these traces, the spectrometer settings are optimized to observe E′ centers. Note the clear generation of an E′ spectrum during stress (middle) and its subsequent recovery post-stress (bottom).

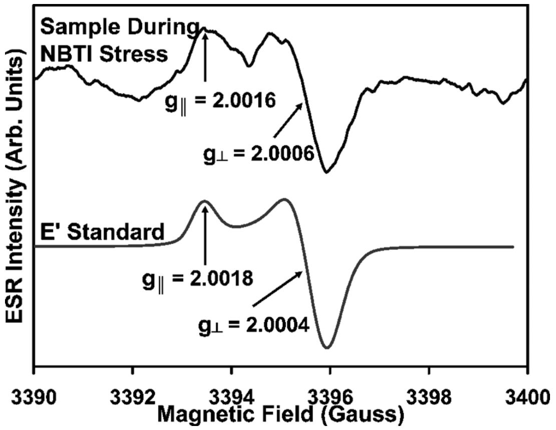

FIG. 4. Comparison of the during NBTI stress spectra from Fig. 3 (top) and a commercially available E′ standard. The standard sample signal to noise ratio is much higher because the standard has orders of magnitude more E′ centers. Note the close correspondence between the g values and line shapes. The gain of the MOS sample trace is approximately 10 000 times higher than used for the E′ standard; all other spectrometer settings are identical. (Note that the precision of g is ±0.0002).

cancy sites (E′ centers) are generated during stress and quickly disappear once the stress is removed. Although the model predicts very fast E′ center recovery, the time resolution of our measurements is slow. We cannot resolve how quickly the recovery occurs.

As mentioned previously, the spectrometer settings used in Fig. 2 were chosen to permit the observation of both Si/SiO$_2$ P$_b$ centers and SiO$_2$ E′ centers and are not optimized for either defect. To further demonstrate that E′ centers (positively charged oxygen vacancy sites) are present during NBTI stressing, Fig. 3 shows three ESR traces taken on the sample before, during and after NBTI stressing. In this figure, the spectrometer settings are optimized for the observation of E′ centers. When NBTI stressing is applied (middle), a clear signal with a powder pattern signal consistent with $g_{\|}=2.0016$ and $g_{\perp}=2.0006$ appears which is characteristic of an E′ center.[9] Upon removal of the NBTI stress (bottom), the E′ signal completely disappears. Figure 4 provides additional evidence linking this signal to an E′ center by comparing the during NBTI stress spectra of Fig. 3 with that of a commercially available E′ standard. Note the close correspondence between the two spectra.

These observations are consistent with and most strongly support the suggestions of Campbell *et al.*[7,8] and Lenahan[11] who suggest that NBTI is triggered by the tunneling of electrons from a neutral E′ center precursor to unoccupied valence band states.[6–8] These results are fully consistent with and support the comprehensive NBTI model of Grasser *et al.*[17] Both the earlier qualitative arguments of Campbell *et al.*,[7,8] Lenahan[10,11] and the more recent quantitative work of Grasser *et al.*[17] point out that the presence of unpassivated E′ silicon dangling bonds in the presence of large numbers of passivated P$_b$ center silicon dangling bonds is thermodynamically unstable. The Gibbs free energy of the P$_b$-H/E′ dangling bond system would be lowered by the exchange of hydrogen from P$_b$-H to E′ dangling bond states, generating interface traps.

Work at Penn State was supported by Texas Instruments through SRC. Part of this work has received funding from the European Community's Seventh Framework Programme under Grant Agreement No. 216436 (project ATHENIS).

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