

D-1-3**Neighboring effect in nitrogen-enhanced negative bias temperature instability**Shyue Seng Tan*, Tu Pei Chen, Jia Mei Soon¹, Kian Ping Loh¹, C. H. Ang², W. Y. Teo² and Lap Chan²

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¹Department of Chemistry, National University of Singapore, Lower Kent Ridge Road, Singapore (119260)²Technology Development Department, Chartered Semiconductor Manufacturing Limited, Singapore (738406)**1. Introduction**

Degradation of p⁺-gate pMOSFETs due to negative bias temperature instability (NBTI) is becoming an increasingly important reliability concern in processes under development and production. Moreover, NBTI is exacerbated by the incorporation of nitrogen into a gate oxide [1]. On the other hand, the effects of nitrogen proximity, fluorine and deuterium have also been reported [1-3]. However, these reports have restricted to process-condition dependence rather than nitrogen concentration dependence. Although it is known that holes and hydrogen are involved in the degradation process [1-3], the role of nitrogen in NBTI has not sufficiently discussed yet. In this paper, we further investigate the nitrogen-enhanced NBTI through experiments and first-principles approach. A quantitative relationship between the threshold voltage shift ΔV_{th} and the interfacial nitrogen concentration N_{int} has been established. The experimental results are further supported by the theoretical calculations of NBTI reaction energies. From these studies, one can conclude that effect of nitrogen in NBTI is two fold. First, it provides more reaction sites. Second, it encourages the NBTI reaction through neighboring effects.

2. Experimental

The devices used in this study were p⁺-gate pMOSFETs with a channel width/length of 10/0.12 μm . Gate oxides with thickness of 1.8 nm were grown by rapid thermal oxidation followed by either *in-situ* rapid thermal nitridation in NO gas ambient or *ex-situ* plasma nitridation. Seven interfacial nitrogen concentrations N_{int} (2.8, 4.5, 5.5, 7.5, 8.5, 12.5 and 15.5 at. %) as determined from secondary ion mass spectroscopy as shown in Fig. 1, were used in this study. NBTI stress was applied to a device at low constant negative gate bias ($V_g = -2.2$ V) under 125 °C. The stress was interrupted at a predetermined period to measure the I-V characteristics.

3. Results and Discussion

Fig. 2 shows the threshold voltage ΔV_{th} as a function of stress time for various N_{int} . For comparison, control sample (i.e. pure SiO₂) is included. This figure clearly spells the nitrogen-enhanced NBTI effect. Figs. 3(a) and (b) shows the increase of midgap voltage shift (ΔV_{MG}) and peak transconductance shift ($\Delta G_{m_{max}}$) after NBTI stress, respectively. Consistent to Fig. 1, nitrogen enhances the degradation. This ΔV_{MG} and $\Delta G_{m_{max}}$ suggest that the degradation is due to creation of the positive fixed charges and interface states, respectively. Fig. 4 depicts the correlation between them and the ΔV_{th} . Evidently, a linear correlation with independent of N_{int} is observed. Therefore,

the degradation of ΔV_{th} , ΔV_{MG} and $\Delta G_{m_{max}}$ are probably due to the same origin of positive fixed charge and interface state generation. The nitrogen concentration dependence of ΔV_{th} under 1000 s NBTI stress is shown in Fig. 5. It is found that ΔV_{th} increases monotonically with N_{int} . In addition, the degradation rate is further accelerated when $N_{int} > 8$ at. %. We could like to attribute this accelerated degradation to N neighboring effect. The details will be addressed below.

To obtain more insight of nitrogen-enhanced NBTI, we performed first-principles study on the impact of nitrogen NBTI reaction at both Si/SiO₂ and Si/SiO_xN_y interface. Fig. 6 shows the various bonding configurations at Si/SiO_xN_y. We confirmed that the our relaxed models give a good representation of the local structure for various bonding configurations by comparing respective bond lengths to previous studies [4-6]. We also calculate reaction energy E_R by subtracting the total molecular energy before reaction from that after the reaction. All calculations were performed using a linear combination of hybrid gradient-corrected density functional theory method.

Fig. 7 shows the reaction energies of NBTI reaction at Si/SiO₂ and Si/SiO_xN_y interfaces. Note that reactions (i) and (ii) have been proposed by previous studies [1,7-8] to explain nitrogen-enhanced NBTI effect. Here, Si₃-Si-H is the precursor of NBTI. Once it is broken by a hole from inversion layer, interface state (Si₃-Si•) and dissociated hydrogen species (e.g. H⁺) would be generated. After that, H⁺ shall diffuse away from the interface and some of them would be trapped by O or N to generate positive oxide charge (Si-OH⁺-Si or Si-NH⁺-Si). It can be clearly seen from the figure that with a positive E_R , the overall NBTI reaction is an endothermic process. In addition, the results show that the E_R for nitrided oxide interface is lower than that for the pure oxide interface, and the E_R decrease with increasing number of N atoms for the nitrided oxide interfaces. A lower E_R means the reaction is easier to occur. The decrease of E_R is attributed to the N neighboring as a result of increasing the nitrogen concentration N_{int} .

Therefore, the observation in fig. 5 can be suitably explained by the N neighboring effect, which is described in the following. A bond structure where one of the four surrounding O atoms is replaced by an N atom (i.e. N-Si-O₃) is dominant when N_{int} is less than 8 at. %. However, when N_{int} is further increased to exceed 8 at. %, a structure where two N atoms are bonded to one Si atom (i.e. N₂-Si-O₂) emerges and becomes dominant when N_{int} goes beyond 10 at. %. The two-N-atoms structure has lower reaction energy [reaction (iii)], showing the N neighboring effect. The above analysis coincides excellently with previous study [8] that N₂-Si-O₂ start to emerge at 8 at. % and dominate when N_{int} goes beyond 10 at. %.

4. Conclusion

In conclusion, for the first time, we have demonstrated the neighboring effect in nitrogen-enhanced NBTI. From the NBTI experiments, it is observed that below 8 at. %, both interface state generation and positive fixed charge increase linearly with interfacial nitrogen concentration. This can be attributed to introduction of nitrogen trap center which lowering the reaction energies of hydrogen trapping. Above 8 at. %, the generation rate is further enhanced and can be understood in terms of the neighboring effect on reaction energies for the NBTI reaction at the interface. Finally, one can conclude that the role of nitrogen is two-fold in oxide. First, it brings more trapping sites. Second, it enhances reactions through neighboring effects. This study

demonstrates that NBTI can be detrimental to future CMOS technology scaling since higher nitrogen content is needed for suppression of boron penetration and gate leakage reduction.

References

- [1] N. Kimizuka *et al.*, *Symp. on VLSI Technology*, p. 92 (2000).
- [2] S. S. Tan *et al.*, *Jpn. J. Appl. Phys.*, **41**, 1031 (2002).
- [3] C. H. Liu *et al.*, *IEEE IEDM Technology Digest*, p. 861 (2001).
- [4] G. M. Rignanese *et al.*, *Phys. Rev. Lett.* **79**, 5174 (1997).
- [5] S. Jeong and A. Oshiyama, *Phys. Rev. Lett.* **86**, 3574 (2001).
- [6] C. G. Van de Walle, *Phys. Rev. B* **49**, 4579 (1994).
- [7] S. S. Tan *et al.*, *Appl. Phys. Lett.* **82**, 1881 (2003).
- [8] J. Ushio *et al.*, *SSDM*, (2001) p. 158.
- [9] T. Hori, *Gate Dielectrics and MOS ULSIs*, (1997) p.232.

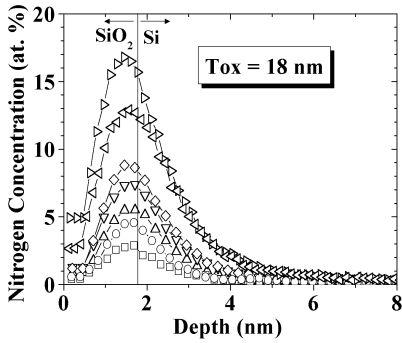


Fig. 1 Depth profiles of nitrogen as determined from secondary ion mass spectroscopy measurement for various nitridation conditions.

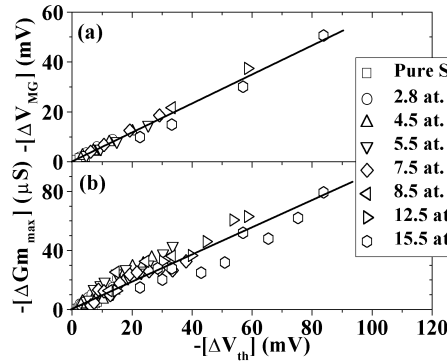


Fig. 4 Correlation between ΔV_{th} and (a) ΔV_{MG} and (b) $G_{m_{max}}$. A linear correlation was found for both cases.

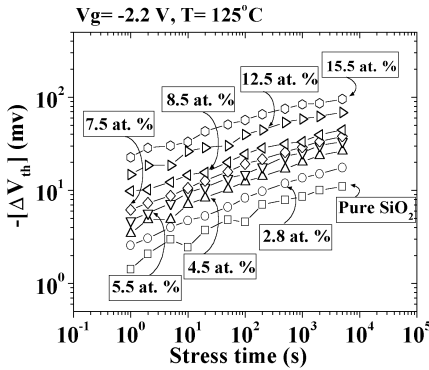


Fig. 2 Increased of V_{th} shift due to NBTI for various N_{int} . This clearly depicts the nitrogen-enhanced NBTI effect.

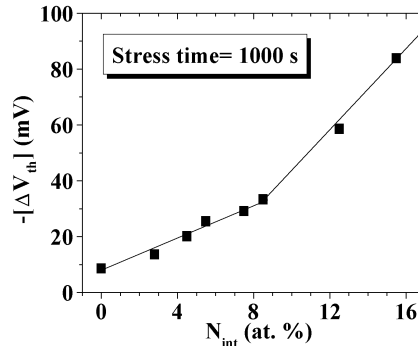


Fig. 5 Dependence of ΔV_{th} on the N_{int} . A constant nitrogen enhancement factor holds up to 9 at. % and increases after 9 at. %.

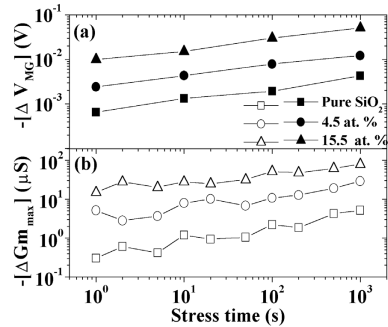


Fig. 3 Decreased of (a) ΔV_{MG} and (b) $\Delta G_{m_{max}}$ due to NBTI for various N_{int} .

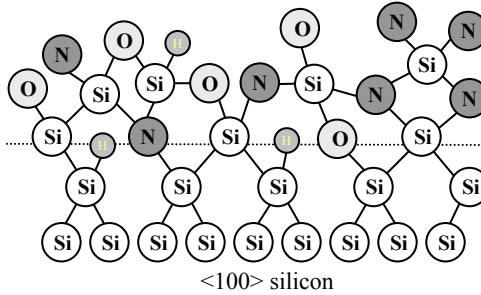
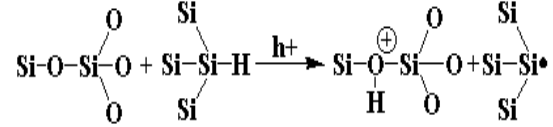


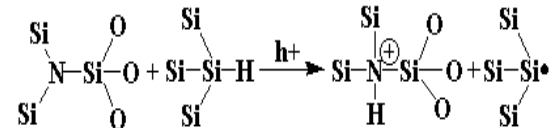
Fig. 6 Bonding configurations of the SiO_xN_y/Si interface.

NBTI reaction at various interface structures

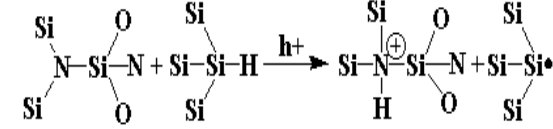
Si/SiO₂ interface: (i). $E_R = 8.84$ eV



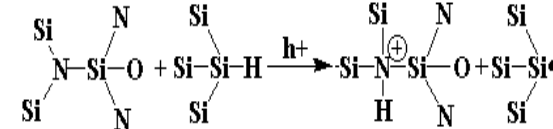
Si/SiO_xN_y interface: (ii). $E_R = 7.81$ eV



(iii). $E_R = 7.65$ eV



(iv). $E_R = 7.46$ eV



(v). $E_R = 7.34$ eV

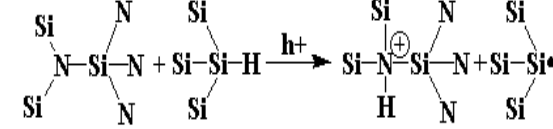


Fig. 7 Reaction energies (E_R) of NBTI reaction at Si/SiO₂ [reaction (i)] and SiO_xN_y [reactions (ii), (iii), (iv) & (v)]. E_R is obtained from first-principle calculations after performing geometry optimization on both reactants and products.