Modeling of Negative Bias Temperature Instability

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After its discovery nearly forty years ago,[1] negative bias temperature instability (NBTI) has again moved to the center of scientific attention as a significant reliability concern for highly scaled pMOSFETs.[2,3] The concern stems from the large number of unsaturated dangling bonds (P_b centers[4]) at the Si/SiO_2 interface, which have to be passivated in order to avoid trapping levels in the bandgap. This passivation is normally achieved by some sort of hydrogen anneal[2] resulting in electrically inactive P_b centers (P_bH). Although the P_bH bonds are very stable, at elevated temperatures and higher electric fields they can be broken, thus reactivating the P_b centers and introducing positive oxide charges. As a consequence, a shift in device parameters is observed, for instance in the threshold voltage and subthreshold slope in MOS devices.[2,3] Most investigations show that P_b centers are essentially involved, however, a universally accepted theory of NBTI is still missing. While earlier work focused mostly on refining the classic reaction-diffusion model of Jeppson and Svensson,[5–7] recently a variety of other explanations have been put forward.[3,8–10] The most likely mechanisms leading to NBTI will be reviewed in the following with special attention paid to modeling issues.

Most degradation mechanisms reported in the context of NBTI are closely linked to hydrogen. Hydrogen in semiconductors is amphoteric and occurs for instance as H^0, H^+, and H_2. Although H^0 is unstable at room temperature[11] and dimerizes within a fraction of a second,[12] it occurs as a transient quantity during various reactions. Depending on process conditions, H^+ can be either extremely stable or highly reactive.[13] A proper understanding of hydrogen in SiO_2 and Si is thus essential.[11] Matters become further complicated due to the various interactions of hydrogen species with dopands[14] and some additional effects occurring for instance in nitrided oxides.[15,16]

The central mechanism in NBT degradation is the dissociation of P_b centers located at the Si/SiO_2interface, most possibly through reactions like

$$P_bH \underset{k_{1r}}{\overset{k_{1f}}{\rightleftharpoons}} P_b + H^0 \tag{1}$$

$$P_bH + H^0 \underset{k_{2r}}{\overset{k_{2f}}{\rightleftharpoons}} P_b + H_2 \tag{2}$$

The forward reaction in (1) is commonly assumed to be the dominant dissociation mechanism. Although the reverse reaction, which is responsible for the passivation through atomic hydrogen, is highly effective, its total impact is normally insignificant[17] due to the low concentration of H^0. However, for the special case of radiation environments, where large quantities of atomic hydrogen are generated in the oxide, and for hot carrier effects it is important.[18,19] This also explains the dual behavior of hydrogen as being able to passivate (k_{1r}) and to depassivate (k_{2f}) dangling bonds. The reverse reaction through H_2 (k_{2r}) *without* preliminary cracking[17] is normally assumed to be the dominant reaction in the case of NBT stress. In an extension of the classical reaction-diffusion (RD) model,[5,6] H^0 is assumed to quickly (instantaneously) dimerize into H_2 which then diffuses away to the p-Si gate.[20,21] Activation energies for the first-order reaction given through k_{2r} were traditionally estimated to be around 1.6 eV. Recent work has shown that although the first-order kinetics can be confirmed, a Gaussian distribution of k_{2r} around 1.5 eV with a standard deviation of 0.15 eV[22,23] has to be considered. This issue has been shown to be important for NBTI modeling.[24,25]

Based on first-principles calculations, the dissociation of P_bH through H^+ has been suggested as the dominant reaction,[10] thereby replacing reaction (1).

$$P_bH + H^+ \underset{k_{3r}}{\overset{k_{3f}}{\rightleftharpoons}} P_b^+ + H_2 \tag{3}$$

The required H^+ is provided through broken PH bonds in the silicon bulk inversion layer. After overcoming the migration barrier at the interface, some H^+ diffuses along the interface before depassivating P_b centers. Alternatively, some H^+ can surmount the energy barrier towards the SiO_2 where they quickly drift to the gate due to the strong electric field.

Another interesting issue is the creation or modification of defects by diffusing hydrogen. Some investigations report that roughly the same number of positive fixed charges as depassivated P_b centers are created,[26] while others attribute NBTI induced V_{th} shifts totally to depassivated P_b centers,[27] provided proper stressing conditions are chosen ($E_{ox} < E_{crit}$). Most positive charges are located close to the interface and have been identified as E' centers (thermal oxide hole traps).[12] E' centers have been reported to dominate oxide hole trapping with their density being strongly process dependent.[12] It has been shown that E' centers react rapidly with H_2, even at room temperature, turning them into hydrogen complexed E' centers (E'H) according to[17]

$$H_2 + E' \underset{k_{4r}}{\overset{k_{4f}}{\rightleftharpoons}} E'H + H^0 \tag{4}$$

In addition, trapping of H^0 has been reported[28]

$$H^0 + E' \underset{k_{5r}}{\overset{k_{5f}}{\rightleftharpoons}} E'H \tag{5}$$

Of particular interest in the case of NBTI is the annealing of E' centers through H_2, which was reported to bring up roughly the same amount of P_b centers,[12] possibly through the following reaction, with H_2 formally being a catalyst.

$$P_bH + H_2 + E' \rightleftharpoons P_b + H_2 + E'H \tag{6}$$

The atomic hydrogen released in the various reactions is commonly assumed to either quickly dimerize into H_2 and diffuse towards the poly gate,[27,29] assuming classical diffusion, or to move dispersively as H^+.[9,30] Dispersive transport models were first applied to describe the movement of holes in amorphous materials[31] and H^+ after irradiation damage.[32] While the first studies were based on the continuous time random walk theory developed by Scher and Montrol,[31,32] multiple trapping models were proposed soon afterwards.[33] Both models exhibit similar features[34] and simplified versions allowing for closed form solutions were used to describe NBTI.[9,30]

Hydrogen motion in the silicon bulk is normally neglected. This might be justified in the case of H_2 based models by the large diffusion barrier found in theoretical studies,[35] or in the case of H^+ by the negative bias driving the protons towards the gate. A frequently cited argument,[20] that two-sided diffusion leads in principle to the same time evolution is likely too simple, since the diffusion coefficients of H_2 in Si and SiO_2 are unlikely to be the same. In addition this would imply, that the same amount of hydrogen species is created on both sides of the interface, which is not plausible considering the different activation energies and the field dependencies.[29,36] Provided that the breaking of PH bonds in the Si bulk is an important source of H^0 and H^+,[10] transport in Si must be included in a rigorous model.

An important issue that has only been approximately dealt with is the behavior of the hydrogen species when they encounter the SiO_2/p-Si interface. Commonly, simplified boundary conditions to the diffusion equation are assumed, either perfect reflection,[6,37] perfect absorber,[6] or perfect transmitter[29] (no trapping). However, a rigorous treatment has to consider the energy barriers,[35] the creation of P_b centers,[38] and re-emission of hydrogen on the p-Si side, analogous to the Si/SiO_2 interface and models used in process-simulation.[39]

NBTI is commonly assumed to be a one-dimensional process,[40] which is in agreement with many reported results, while only the closely related damage caused by hot-carrier injection is acknowledged to require a two-dimensional treatment of the diffusion equation. Even if all processes leading to NBTI were one-dimensional, inhomogeneous doping profiles,[41] variable oxide thicknesses such as found in HV devices, or inhomogeneous stress conditions ($V_\mathrm{DS} \neq 0$)[41] require a two-dimensional description of the problem. Even for homogeneous stress ($V_\mathrm{DS} = 0$) a gate length dependence is occasionally reported,[2] which can be modeled by allowing diffusion of H^+ along the interface as observed experimentally[42] and confirmed theoretically.[13]

A commonly neglected issue in NBTI modeling is the coupling of the 'hydrogen equations' to the semiconductor device equations. Obviously, the dynamical creation and annihilation of P_b and E' centers influences the electric field distribution and thus the reaction rates and the transport properties. This issue is of particular importance when annealing during measurements[43] is to be understood. Some issues need to resolved when such a coupling is attempted. First, the charge trapped in the amphoteric P_b centers depends on the position of the Fermi-level and thus on the bias conditions. To model this effect, the density of created P_b centers needs to be coupled to the electrically active interface trap density-of-states $D_\mathrm{it}(\mathcal{E})$ in a surface recombination process.[44] A lot of information on D_it is available and it is known that in addition to be band-tail states P_b centers introduce two distinct peaks in the Si bandgap.[4,19] The shape of these peaks has been described using Fermi functions[45] where the two peak values evolve differently in time with each width staying roughly constant.[12,19] Regarding the contribution of trapped holes in the oxide, precise statements on where exactly these charges are located are important to properly model the shape of the band-edges in SiO_2, which directly influence the oxide field and thus charge carrier transport and tunneling rates.

A specific coupling issue concerns the influence of holes which are commonly assumed to be 'available'. The dissociation rate k_1f is often assumed to depend on the concentration of the inversion layer holes, a quantity not directly available in NBTI models. Here, a rigorous coupled solution can provide better estimates. Although the importance of holes in this process is widely acknowledged, the mechanisms have not yet been evaluated rigorously and it is not clear whether the rate is determined by the hole concentration itself or whether the presence of holes modifies the activation energies.

Although significant progress regarding the understanding of NBTI has been made in the last decade, a universal 'one-fits-all' model is still a hot topic of research.

[1] E. Deal *et al.*, J.Electrochem.Soc. **114**, 266 (1967).
[2] D. Schroder *et al.*, J.Appl.Phys. **94**, 1 (2003).
[3] V. Huard *et al.*, Microelectr.Reliab. **46**, 1 (2006).
[4] E. Poindexter *et al.*, J.Appl.Phys. **56**, 2844 (1984).
[5] K. O. Jeppson *et al.*, J.Appl.Phys. **48**, 2004 (1977).
[6] S. Ogawa *et al.*, Phys.Rev.B **51**, 4218 (1995).
[7] M. Alam, in *Proc. IEDM* (2003), pp. 345–348.
[8] S. Zafar, J.Appl.Phys. **97**, 1 (2005).
[9] B. Kaczer *et al.*, Appl.Phys.Lett. **86**, 1 (2005).
[10] L. Tsetseris *et al.*, Appl.Phys.Lett. **86**, 1 (2005).
[11] C. Van de Walle *et al.*, IEEE Trans.Electr.Dev. **47**, 1779 (2000).
[12] P. Lenahan *et al.*, J.Vac.Sci.Technol.B **16**, 2134 (1998).
[13] S. Rashkeev *et al.*, Appl.Phys.Lett. **81**, 1839 (2002).
[14] C. Van de Walle *et al.*, Phys.Rev.B **39**, 10791 (1989).
[15] M. Denais *et al.*, in *Proc. IRW* (2004), pp. 121–124.
[16] D. Ang *et al.*, IEEE Electron Device Letters **26**, 906 (2005).
[17] K. L. Brower, Appl.Phys.Lett. **53**, 508 (1988).
[18] E. Cartier *et al.*, Appl.Phys.Lett. **63**, 1510 (1993).
[19] E. Cartier *et al.*, Appl.Phys.Lett. **69**, 103 (1996).
[20] S. Chakravarthi *et al.*, in *Proc. IRPS* (2004), pp. 273–282.
[21] D. Varghese *et al.*, in *Proc. IEDM* (2005), pp. 1–4.
[22] A. Stesmans, Appl.Phys.Lett. **68**, 2076 (1996).
[23] A. Stesmans, Phys.Rev.B **61**, 8393 (2000).
[24] M. Houssa *et al.*, Appl.Phys.Lett. **81**, 709 (2002).
[25] V. Huard *et al.*, Microelectr.Reliab. **45**, 83 (2005).
[26] M. Denais *et al.*, in *Proc. ESSDERC* (2005), pp. 399–402.
[27] S. Mahapatra *et al.*, Microelectr.Eng. **80**, 114 (2005).
[28] D. Griscom, J.Appl.Phys. **58**, 2524 (1985).
[29] M. Alam *et al.*, Microelectr.Reliab. **45**, 71 (2005).
[30] M. Houssa *et al.*, Appl.Phys.Lett. **86**, 1 (2005).
[31] H. Scher *et al.*, Phys.Rev.B **12**, 2455 (1975).
[32] D. Brown *et al.*, J.Appl.Phys. **70**, 3734 (1991).
[33] V. Arkhipov *et al.*, Philos.Mag.B **45**, 189 (1982).
[34] V. Arkhipov, in *Proc. ISEIM* (1995), pp. 271–274.
[35] L. Tsetseris *et al.*, Phys.Rev.B **70**, 1 (2004).
[36] J. Ushio *et al.*, J.Appl.Phys. **97**, 1 (2005).
[37] H. Aono *et al.*, Microelectr.Reliab. **45**, 1109 (2005).
[38] M. Houssa, Microelectr.Reliab. **45**, 3 (2005).
[39] F. Lau *et al.*, Appl.Phys.A **49**, 671 (1989).
[40] H. Kufluoglu *et al.*, in *Proc. IEDM* (2004), pp. 113–116.
[41] C. Schlünder *et al.*, Microelectr.Reliab. **45**, 39 (2005).
[42] R. Stahlbush *et al.*, IEEE Trans.Nucl.Science **41**, 1844 (1994).
[43] M. Denais *et al.*, in *Proc. IEDM* (2004), pp. 109–112.
[44] W. Eades *et al.*, J.Appl.Phys. **58**, 4267 (1985).
[45] A. Haggag *et al.*, in *Proc. IRPS* (2001), pp. 271–279.