Experimental and theoretical studies of negative bias temperature instability in ultra-thin gate dielectrics

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Experimental and Theoretical Studies of Negative Bias Temperature Instability in Ultra-thin Gate Dielectrics

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Summary

It has been the intent of this work to investigate negative bias temperature instability of pMOSFET with ultra-thin gate dielectrics both theoretically and experimentally. Through experimental study, a comprehensive and quantitative study on the influence of nitrogen at the Si/SiO_xN_y interface on NBTI has been presented and several features regarding the nitrogen-enhanced are unveiled. Based on the findings established from experimental works, an atomic model of NBTI is developed using first-principles calculations. In the model, the possible origin of NBTI in both SiO₂ and nitrided oxides are discussed. In addition, the effect of nitrogen as a i) reaction site and ii) neighboring atom in NBTI are discussed. Consequently, the role of nitrogen in NBTI can be understood in terms of its electronegativity, atomic charge distribution and increasing initial interfacial defect density. It has also been successfully demonstrated that interfacial strain and oxide stoichiometry has strong impact on NBTI through experimental and theoretical study. In particular interfacial strain can deteriorate the hydrogen-originated hole trapping reaction. This means the relaxation of the strained-layer at the oxide/Si interface is more requisite issue to improve the reliability and to realize the aggressive scaling. Fortunately, NBTI degradation in actual AC operation environment can be relaxed. This is because some NBTI-induced defects can be annealed when the stress is removed or when the device is in OFF mode. The annealing effect is attributed to reverse reaction. To accurately extract the device lifetime from the static measurement, a dynamics lifetime model has been developed. Consequently, another comparison on the three types of digital waveforms is carried out and their impact on degradation is discussed. For the study of NBTI on high-k gate dielectrics, it is found that Group IVB

pure metal oxide has higher NBTI immunity than that of Group IIIA/IIIB based high-k and pure SiO₂. Although NBTI immunity of Group IVB silicate based high-k films is slightly worse as compared to their respective pure metal oxides, they still show energetically unfavorable for NBTI. In addition, Group IIIA/IIIB based high-k is a poor candidate for replacement of SiO₂ as far as NBTI is concerned. Furthermore, nitrogen-enhanced NBTI remains a disturbing issue in high-k oxynitride based alloy.

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CHAPTER ONE

Introduction

This thesis is a presentation of research work performed at the Nanyang Technological University. This work is a study of the reliability issue, i.e. negative bias temperature instability (NBTI), in metal-oxide-semiconductor field-effect-transistors (MOSFET) with ultra-thin gate oxides (≤ 3 nm). This chapter introduces the background and the purpose of this work. More details of the work is presented in the following chapters.

1.1 A Brief History of Metal-Oxide-Semiconductor Devices

The concept of a surface field-effect transistor, predecessor of the modern MOSFET, was first proposed as early as the 1930s [1]. It was until the 60's that the silicon technology became mature enough to realize MOS gate stacks based on the thermal SiO₂-Si framework. Followed by the first integrated circuit (IC) invented in 1959 [2], then the large-scale commercialization of MOS technology took place. Today's ultra-large-scale-integration (ULSI) system are built upon the low power consumption, high packing density MOS structure namely the complementary MOSFET (CMOS) proposed in 1963 [3]. The MOSFET has become a device of choice for an array of digital integrated circuits, with microprocessors and DRAMs leading the field. Over the last four decades, the CMOS technology has constantly experienced device scaling towards ever-smaller dimensions (e.g. gate length and gate width), higher device performance and

higher packing density. This has allowed the silicon MOSFET technology to emerge as the prevailing technology for today's ULSI applications.

1.2 MOSFET Scaling

Growth in silicon technology was driven primarily by the need to build MOSFETs that would work faster and more efficiently. To meet this challenge, the MOSFET is continuously being downsized based on a set of guidelines established over the past four decades. For instance, according to Moore's law [4], for every three years, the device dimension is reduced by $1/\sqrt{2}$, the chip size is increased by 1.5 times, and the number of transistors in a chip is increased by a factor of four. By reducing the device dimensions, in particular the transistor gate length can increase the amount of current supplied by a transistor. Higher current allows the circuits to switch more quickly, leading to faster computations. In addition, the reduction in transistor size also allows more transistors to be integrated on a single chip. Consequently the complexity and functionality of ICs can be increased while keeping the cost of the circuit fabrication low. This in turn constantly expands the realm of possible applications of semiconductor products.

Scaling down the device dimension enforces other changes in the MOSFET design in order to keep it operational at the scaled geometry. Therefore, scaling a MOSFET involves all aspects of the MOSFET technology, such as lithography, etching, power supply voltage, threshold voltage, short-channel effects, gate dielectric thickness, high field effects, dopant density fluctuation, interconnect delays, device reliability and novel device structures [5]-[7]. Traditionally, downsizing has been paced by the development of new lithography tools, masks, photoresist materials and critical dimension etch processes. In the past several years, it has become clear that despite

advances in these crucial technologies and the resultant ability to produce ever-smaller feature sizes, front-end technologies have not kept pace, and device performance has been compromised. The crux of this problem comes from the fact that the traditional gate dielectric film has been pushed to fundamental material limits and continued scaling has required modification of the materials or introduction of new materials.

1.3 Issues with gate dielectric scaling and motivation

Silicon dioxide (SiO_2) has been the gate dielectric of choice since 1960, when it was first proposed that thermally grown SiO_2 should be used as the gate insulator in the MOSFETs [8]. Research, development and production over the past four decades have shown SiO_2 to exhibit superior interfacial properties and to provide excellent passivation of the silicon surface from contamination. This is due to the fact that nature has endowed SiO_2 with many unique and outstanding properties. For instance, SiO_2 is native to Si, and thus forms an interface with low defect density ($\sim 10^{10} \text{ eV}^{-1} \text{ cm}^{-2}$, after H_2 passivation). Meanwhile SiO_2 has high resistivity ($\sim 10^{15} \Omega \text{ cm}$), excellent dielectric strength ($\sim 1 \times 10^7 \text{ V/cm}$), and a large band gap ($\sim 9 \text{ eV}$). All these properties are in large part responsible for enabling the microelectronics revolution.

Progress in silicon IC technology has been dominated by the reduction in gate length to increase device performance and integration. To keep pace with drive current demands and better gate control over the channel, the gate dielectric thickness must also scale in accordance with the gate length. As can be seen from Fig. 1.1, gate dielectric thickness continues to shrink aggressively to offer higher drive current and gate capacitance required by scaled MOSFETs. The term *equivalent* oxide thickness refers to the physical thickness of the dielectric multiplied by the ratio of the permittivity of pure

Figure 1.1: Decrease in gate SiO_2 (or equivalent oxide) thickness with device scaling (technology generation). Actual or expected year of implementation of each technology generation is indicated [Extracted from ITRS (Ref. 9)].

SiO_2 to that of the dielectric film. The use of ultra-thin gate oxide, although very promising for high performance MOSFETs, still remains a critical research topic, for its qualification for the next-generation of devices. Related to the employment of ultra-thin oxides, the following issues need to be resolved:

- (i). Direct tunneling current (DT)
- (ii). Boron penetration and gate poly-silicon depletion
- (iii). Quantum mechanism effects
- (v). Integration issue and manufacturability
- (iv). Oxide Reliability

1.3.1 Direct tunneling current (DT)

Instead of tunneling into the conduction band of the SiO_2 layer like Fowler-Nordheim (F-N) tunneling, electrons can tunnel directly through the forbidden energy gap of the SiO_2 layer, which is the so-called “direct tunneling”. Different from F-N tunneling, carriers in DT tunnel through a trapezoidal barrier, the tunneling distance does not vary with the oxide field. As a result, DT current shows a distinct characteristic of a lesser dependence on oxide field than F-N tunneling. However, as thickness of the oxide layer decreases as part of scaling requirements, the DT current increases approximately in an exponential manner. In deep submicronmeter MOSFETs, the gate oxide has been scaled to below 2 nm. For such an ultra-thin oxide, a significant DT current is expected to be observable even at normal operating voltage. The most prominent impact of direct tunneling current is to greatly increase the power consumption of a chip. It is thereby one of the limiting factors for CMOS scaling.

1.3.2 Boron penetration and gate poly-silicon depletion

Both boron penetration and poly-silicon depletion effect are more pronounced in p^+ -gate pMOSFET than n^+ -gate nMOSFET. Dopant depletion occurs due to non-uniform dopant distribution in the gate electrode such that a thin layer of depletion forms during channel inversion. Ultimately, this thin depletion layer decreases the total gate capacitance and lower device speed. Industry has been increasing the gate implant dose to suppress this depletion effect. However, boron penetration through the ultra-thin gate oxide occurs and alters the device threshold voltage. Therefore, nitrogen is introduced into SiO_2 to suppress the boron penetration effect. The tradeoff between poly-silicon

depletion and boron penetration is the major hurdle for the ultra-thin gate dielectric film, which has emerged with scaling in ULSI.

1.3.3 Substrate quantum mechanism (QM) effects

As part of scaling, oxide thickness is reduced and the substrate doping concentration is increased to suppress short-channel effects. However, the supply voltage is less aggressively scaled than the gate oxide thickness. As a result, the operating electric field over the oxide becomes higher. Due to this higher electric field, which is perpendicular to the Si surface, the energy band is bent strongly near the semiconductor-oxide interface. A potential well is thus formed by the oxide barrier and the electrostatic potential in the semiconductor. Instead of three-dimensional continuous energy states in classical physics, from the quantum mechanical point of view, the electrons are confined in this potential well, forming discrete subbands called quantization. The QM effect results in reduction of overall gate capacitance and cause the threshold voltage to increase. As a consequence, the transistor speed enhancement is compromised as further scaling of the transistor is pursued.

1.3.4 Fabrication and manufacturability

From the processing point of view, it is increasingly difficult to grow a uniform ultra-thin oxide layer, e.g. 1.2 nm of SiO₂ only 4 monolayers thick, not to mention a perfect stoichiometry for such an ultra-thin layer. Non-uniform dielectrics can also further enhance the tunneling current and provide a rough interface. This poses a serious challenge to the gate oxide fabrication process.

1.3.5 Oxide reliability

Figure 1.2: Oxide electric field E_{ox} as a function of time for CMOS circuits.

Oxide degradation and breakdown have received increasing attention since they cause failures in advanced ULSI devices and, therefore, may impede the downscaling trend of oxide thickness and MOSFET size [10]-[12]. This is partly due to the fact that the scaling of supply voltage is less aggressive, resulting in an increasing oxide field E_{ox} , as depicted in Fig. 1.2. In addition, the charge-to-breakdown decrease with decreasing oxide thickness due to the reduction of the critical defect density that leads to oxide breakdown under constant voltage stress [13]. With these concerns, the reliability of ultra-thin gate dielectrics has become another limiting factor for future ULSI development. Another critical issue that is associated with oxide scaling is negative bias temperature instability (NBTI). In recent years, it has been widely recognized that NBTI renders the fabrication of highly reliable p-channel MOSFET (pMOSFET) unfeasible [14],[15]. It could shift the threshold voltage (ΔV_{th}) by as much as 50 – 100 mV in a pMOSFET over a period of months to years, depending on the operating condition of a chip. As a consequence, it

would be more difficult to turn on the pMOSFET, causing a significant reduction in circuit speed.

1.3.6 Motivation

Many of the above issues still remain a challenge. In particular, we look into the NBTI issue in pMOSFET in this research project. This is because for the past few years, there has been an evolutionary change in the lifetime limiting factor for CMOS technology, as a result of the NBTI issue in the pMOSFET. Traditionally, for 0.35 μm technology and above, hot-carrier injection (HCI) induced degradation of n-channel MOSFETs limits the lifetime of CMOS circuitry, and therefore considerable works have been made to understand the mechanism responsible for defect generation in nMOSFETs under HCI stress [14]. However, with aggressive scaling of the thickness of gate oxide film into the direct-tunneling regime, NBTI degradation in pMOSFETs, instead of the HCI degradation in nMOSFETs, limits the CMOS lifetime [14]. Over the last few years, it has been established that the nature of dielectric degradation in ultra-thin oxides is fundamentally different from that in thicker oxides. Therefore, reliability issues like NBTI need to have their physics re-examined when the gate dielectric thickness is reduced to barely several atomic layers.

Another challenge is that the NBTI reliability physics of ultra-thin gate dielectric become even more complicated especially when continued scaling has required mandatory modification like incorporation of nitrogen into the SiO_2 film to form silicon oxynitride (SiO_xN_y). It is thus necessary to study in detail the role of nitrogen on the NBTI degradation of SiO_xN_y film, as such a study is still largely lacking.

Further reduction in oxide thickness to a few monolayers, however, exacerbates the reliability degradation. One of the critical problems is related to the strain/stress at the oxide/Si interface and the stoichiometry of the oxide, due to the fact that their impacts become more apparent in ultra-thin oxide films. There is still no study devoted to understand the effects of strain and stoichiometric oxide on NBTI despite their importance in the ultra-thin gate dielectric. This is partly because of the lack of techniques to formulate the experiment.

Besides, there are even more profound reliability challenges associated with the implementation of the high-k dielectric film. This is because employment of such a high-k gate dielectric is expected by 2007 to suppress the increasing direct tunneling current in the ultra-thin SiO₂ layer. Therefore, understand the mechanism in NBTI in high-k dielectric is crucial prior to their implementation [9].

The semiconductor industry is poised for a paradigm shift in Moore's Law and technology scaling in the next 5 years, if the impact of NBTI and other key issues on the performance of MOSFETs is not addressed. The pressure to maintain the roadmaps outlined above will continue to increase, but without addressing these secondary issues, fabrication facilities may not be able to deliver competitive products. Second, designers are now under extensive economic pressure to have their designs work the first time. Therefore, the ability to tackle these issues will make the difference between having a highly profitable product versus an uncompetitive high-loss product.

In short, all the above factors form the major motivation of this research work, which addresses the issue of NBTI in the ultra-thin gate dielectric of the pMOSFET.

1.4 Objectives and approach

A thorough understanding of the degradation processes, which are responsible for the long-term degradation of the device characteristics, is naturally the first prerequisite for building accurate simulation models, and for evaluating the device-level and circuit-level damages associated with these processes. Traditionally, understanding the reliability physics of the Si/SiO₂ technology has relied heavily upon experimental approach. This approach has two drawbacks. Firstly, the success of this approach on understanding the Si/SiO₂ reliability physics can largely be attributed to the extensive data and insight gained from many decades of experimental work on the system. Hence, the time and cost of acquiring such an extensive knowledge database for the system are extremely expensive. Secondly, it cannot provide accurate atomistic behavior of the system. Understanding the atomistic behavior of the system is essential in order to manipulate the properties of novel materials.

In contrast, atomic scale modeling, which includes atomistic and quantum simulations, can accurately predict material properties based on the microscopic interactions between atoms, in the case of atomistic simulation, or between electrons, in the case of quantum simulation. Atomic scale modeling is then a promising way to fill the voids in the reliability knowledge of gate dielectrics, and predicting their microscopic behavior. Furthermore, atomistic modeling can be considered in the situation where experiment is impossible or extremely difficult to manipulate. This principle is not limited to situations that are completely inaccessible to experiment, but also includes the performance of “computational experiments,” which afford far greater “experimental” control than their physical counterparts. For instance, one can “reach into” a theoretical calculation and, at will, bend chemical bonds at experimentally unstable and inaccessible

angles to gain insight into the processes controlling the reactions. Or, one can study the properties of isolated defects in a material, in which the segregation of impurities towards these defects tends to cloud the experimental results.

Nevertheless, one cannot totally ignore experimental work because it can provide some hints to the underlying reactions. Therefore, there are three major goals for this research, which encompass both atomistic modeling and experimental work. First, it is aimed at obtaining a better understanding of NBTI in ultra-thin gate dielectrics. To accomplish this goal, we first fabricated several ultra-thin gate oxides at different processing conditions, e.g. nitridation temperature and time, annealing ambience, etc. to gather information on the species involved in NBTI. Next, we performed first-principles calculation to investigate the possible atomistic reactions that occur during NBTI. Finally, we aim to propose possible solution to suppress NBTI. The second objective is targeted at understanding the effects of strain and stoichiometry of the oxide on NBTI using first-principles calculations. The last objective is aimed at investigating and understanding the NBTI resistance of high-k gate dielectric films. Ultimately, the scope of this thesis work is centered on the study of NBTI in the pMOSFET, using both theoretical and experimental approaches.

1.5 Major contribution of the Thesis

The major contributions of this research are listed below.

- 1). Establish a qualitative relationship between interfacial nitrogen and NBTI thermal activation energy. The role of nitrogen has been confirmed to have insignificant impact on the time exponent factor and oxide field dependence of NBTI [15].
- 2). Perform pioneering work on plasma nitridation to suppress the nitrogen-worsen

NBTI effect [16], [17].

- 3). Demonstrate the effect of nitrogen profile engineering on NBTI and establish that nitrogen at the Si/SiO_xN_y interface plays a significant role on NBTI degradation while nitrogen in the bulk oxide have a trivial role [18].
- 4). Propose that nitrogen-worsen NBTI effect is related to the enhanced trapping of released hydrogen species at N bridging atoms than that at O bridging atoms [19].
- 5). Establish a linear relationship between the released hydrogen (H⁺) trapping reaction energy and NBTI-induced defect generation [20].
- 6). Demonstrate that the neighboring N atom at the positive oxide charge trapping center can further deteriorate the nitrogen-worsen NBTI effect [20], [21].
- 7). Investigate the effect of topology modification, as a result of nitrogen incorporation, on Si-H bond energy and vacancy formation and their implication on NBTI [22].
- 8). Propose the importance of interfacial strain on NBTI through experimental finding and confirm the proposal through first-principles calculation. In addition, the relationship between interfacial strain and nitrogen-worsen NBTI is elucidated [23].
- 9). Investigate the NBTI in dynamic stressing mode and confirm that NBTI-generated defects can be partially annealed when the stress is removed [24].
- 10). Propose a new lifetime model for dynamic NBTI in an inverter circuit [25].
- 11). Propose the annealing effect in dynamic NBTI is due to the reverse reaction, which is re-passivation of both positive oxide charge and interface traps [26].
- 12). Investigate and compare the immunity of various high-k gate dielectric films to the hydrogen-originated hole trapping reaction (NBTI) [27].

1.6 Organization of the Thesis

This thesis investigates the mechanism of negative bias temperature instability through the use of experimental work and first-principles density functional theory calculations. The thesis is organized as follows:

Chapter 2 reviews some of the previously proposed NBTI models. The advantages and drawbacks of each model are discussed. In addition, the effects of various processing conditions on NBTI are reviewed. This chapter also describes the theories of atomistic models that we employ to develop the atomic model of NBTI. The characteristics of the two main approaches, classical models and quantum mechanical models are discussed. Based on the requirements for NBTI modeling, quantum mechanical-density functional theory is identified as the most promising method for its atomic reaction of interest.

Chapter 3 presents a comprehensive and quantitative study on the influence of nitrogen at the Si/SiO_xN_y interface on NBTI. Detailed analysis of the nitrogen effect under various stressing conditions leads to several conclusions that help us better understand the role of nitrogen in NBTI. Based on the understanding of NBTI, plasma nitridation is introduced to suppress NBTI-induced degradation.

Chapter 4 describes atomic modeling of NBTI in SiO₂ and SiO_xN_y gate dielectrics using first-principles density-functional calculations. With the aid of experimental findings in Chapter 3 and other reported work, we develop the NBTI atomic model.

Chapter 5 employs experimental and theoretical studies to demonstrate the impact of interfacial strain and oxide stoichiometry on NBTI. It is confirmed that interfacial strain has a strong impact on NBTI. Therefore, the relaxation of the strained-layer is requisite to improving reliability and to realizing aggressive scaling.

Chapter 6 focuses on an important aspect of NBTI in the PMOS transistor, namely dynamic NBTI, and aims to develop an efficient and reasonably accurate lifetime model to facilitate dynamic lifetime extraction from static measurement. It is found that the NBTI-induced degradation is partially annealed when the stress is removed. The mechanism of the annealing effect is proposed to be the reverse reaction of NBTI. Consequently, a comparison on the three types of digital waveforms is carried out and their impact on degradation is discussed.

Chapter 7 investigates and compares the NBTI immunity of various potential high-k films. It is found that Group IVB metal oxide has higher NBTI immunity than that of Group IIIA/IIIB based high-k and pure SiO₂. However, nitrogen-worsen NBTI remains a disturbing issue in high-k oxynitride based alloys.

Chapter 8 summarizes the work presented in this thesis. Finally, the directions for future work are pointed out.

CHAPTER TWO

Review of NBTI in pMOSFETs and Atomistic Modeling

This chapter reviews some of the NBTI models proposed previously for interface trap and positive oxide charge generation. The advantages and limitations of each model are discussed. In addition, the effects of various processing conditions on NBTI are reviewed. Furthermore, this chapter describes briefly the theories of atomistic models that we employ to develop the atomic model of NBTI.

2.1 Review of NBTI in pMOSFETs

Research on NBTI can be traced back to the very early days of MOS device development, having been observed as early as in 1967 by Deal *et al.* [28], [29]. They found that both the interface trap density N_{it} (cm^{-2}), Q_{it} ($\text{C}\cdot\text{cm}^{-2}$), or D_{it} ($\text{cm}^{-2}\cdot\text{eV}^{-1}$) and oxide charge density N_{ox} (cm^{-2}), or Q_{ox} ($\text{C}\cdot\text{cm}^{-2}$) increased upon negative bias stress. The rates of increase of both N_{it} and N_{ox} were very similar. In 1973, Goetzberger *et al.* reported the same observation using metal gate devices with 100 nm thick oxides, stressed at -10^6 V/cm at 300 °C [30]. Four years later, Jeppson and Svensson confirmed the observation that there is an equal growth of oxide charge and surface trap density, independent of the BTI stress field and temperature [31]. Their result is shown in Fig. 2.1.

This one-to-one correlation between N_{it} and N_{ox} has also been endorsed and confirmed by many other researchers [32]-[36]. Another common observation is that the generation of interface trap and positive oxide charge follow a power-law time dependence with the exponent having values in the range of 0.20 ~ 0.25 [33]-[37].

Figure 2.1: The increase of the oxide charge measured as the shift of the C-V curve at midband, plotted against the relative surface-trap density at midband. The same relationship is observed after NBS at both 125 °C, -55 V (5.8 MV/cm) and 25 °C, -65 V (6.8 MV/cm) and indicates that there is roughly one surface trap per oxide charge. [Re-plotted using data from Ref. 31.]

2.1.1 NBTI-induced positive oxide charge model

Despite the significant increase in interface trap density, positive oxide charge generation due to NBTI received the most attention in the early days. For instance, Deal *et al.* attributed the charge generation to the field-assisted penetration of positively charged excess silicon atoms into the oxide. Subsequently, various models have been proposed to explain how positive oxide charge is produced during negative bias temperature stressing. The first model is hole trapping, which results from the filling of intrinsic hole traps via holes from the Si substrate [38]-[40]. As can be seen from Fig. 2.2, the translation of C-V curve to the left indicates filling up of intrinsic hole traps, generated during metallization, by NBTI stress.

Figure 2.2: High-frequency C-V curve after room-temperature negative bias temperature stressing for 110 nm dry oxides damaged during electron beam metallization. Film were stressed using a field of -3 MV/cm; (a) 0 s (original C-V curve), (b) 30 s, (c) 210 s, and (d) 1000 s. [Re-plotted using data from Ref. 40]

This model is based on the observation of a significant “charging current” which flows during NBTI and is correlated with the production of positive oxide charge [39], [40]. The second model is thermally assisted electron tunneling, in which the trap centers causing the charge trapping, are either neutral or positive and are distributed throughout the oxide near to the interface [41], [42]. Under the influence of a negative voltage some of the centers are raised above the Fermi level. The charging process is a thermally assisted tunneling process, where electrons in the excited states tunnel into the empty state of the conduction band of silicon, leaving behind a positively charge center as illustrated in Fig. 2.3 [41], [42].

Figure 2.3: Energy diagram of the oxide centers. V_{FB} is the flatband voltage and V_b is the negative voltage bias applied to the gate of the MOS device. (a) Flatband condition: The trapping centers are neutral and the ground states of the centers lie below the top of the valence band of the silicon. The centers have excited states, $E_A \approx 1.3$ eV. (b) Charging of the centers: The negative voltage causes a number of ground states to become positively charged by the thermal emission of electrons to the excited states, from which the electrons can tunnel to the silicon. [Extracted from Ref. 41].

The third model is based on strained bonds in the oxide network, which act as hole traps [43]. This model predicts that relaxation of strained bonds after capture of holes gives rise to trapped positive charge centers that are permanent damage sites in an oxide. Although each of the models is substantiated by a good number of experimental findings, none of the models can elucidate the correlation between the interface trap generation and positive oxide charge generation during NBTI. In addition, none of the models offers a consistent explanation for the universal $t^{0.25}$ time dependence for defect generation.

2.1.2 NBTI-induced interface trap generation model

To explain the interface trap generation, many researchers have unanimously adopted the well-known Si-H dissociation mechanism. In particular, Si-H dissociation is a two-reaction model involving atomic hydrogen dimerization and hydrogen-interface reactions [44]-[46]:

In this scenario, the high electric field dissociates the Si-H bonds, yielding H^0 , a neutral interstitial hydrogen atom or atomic hydrogen. H^0 is highly reactive and is considered a fast diffuser in the oxide [46]. It is possible that the H^0 acts as the promoter of N_{it} generation, as shown in Eq. 2.2 (from left to right), as well as the suppressor of N_{it} generation, as shown in Eq. 2.2 (reverse direction). In addition, the released H^0 will immediately form molecular hydrogen with other available H^0 , as depicted in Eq. 2.3. On the whole, the concentration of H^0 plays an important role in balancing the formation or passivation of interface trap.

Another model that is sometimes used to explain NBTI induced interface trap generation considers the interaction of Si-H bond with holes at Si/SiO₂ interface [33], [47]-[51]. Dissociation involving holes is given by

This possibility is based on the observation that the released hydrogen transports in oxide as H⁺ [52], [53]. It is also consistent with recent results indicating that reverse substrate bias accelerates NBTI degradation [54]. Furthermore, as reported recently, H⁺ is the only stable charge state of hydrogen at the interface [55]. Therefore, another model for N_{it} formation is that H⁺ reacts directly with the Si-H bond to form an interface trap, according to the reaction [55]

It is worth mentioning that these models (i.e. Eqs. 2.4 and 2.5) are consistent with theoretical models that predict lower activation energies for hydrogen dissociation from the Si-H bond when a charged-state exists [56], [57]. In addition, a donor-type interface state has been proposed for BTI degradation to explain why such degradation exists only in pMOSFET but not in nMOSFET [58]. Till now, the hydrogen dissociation model remains the most consistent NBTI-induced interface trap model.

2.1.3 NBTI diffusion electrochemical model

Jeppson and Svensson were the first to propose a comprehensive model for NBTI. They proposed a diffusion-reaction concept to explain the $t^{0.25}$ time evolution of NBTI degradation [31]. In this model, it is assumed that the silicon interface contains a large number of defects (i.e. Si-H bonds), which are electrically inactive, but may become electrically active upon BTI stress. However, in this diffusion reaction model, an assumption of infinite oxide thickness is adopted so that the effect of gate polysilicon-oxide interface could be completely ignored. This treatment is suitable for thick oxide at that time. However, for the ultra-thin gate oxides that are used in current technology, one can no longer ignore the gate polysilicon-oxide effect in this diffusion reaction model. In 1995, the diffusion-reaction model was refined by Ogawa et al. [50] to extend its application to ultra-thin oxides. In this diffusion reaction model, the ubiquitous $t^{0.25}$ is attributed to the following diffusion-limited electrochemical reactions [31], [50]:

where X denotes the diffusion species. When the interface defect like a Si-H bond is electrically activated, the diffusing species leaves a defect site at the Si/SiO₂ interface where an interface state and a positive oxide charge are generated. This model agrees with the observation that equal numbers of interface states and positive oxide charges are produced. At the actual interface, there are a lot of hydrogen-terminated trivalent Si bonds (Si-H), which are inactive in this form. The Si-H bonds have been proposed as the origin for both the oxide charge and interface state generation under NBTI stress. As for possible diffusion species, interstitial atomic hydrogen (H⁰) [44], [45], [48], [59], [60], molecular hydrogen (H₂) [46], [50], [61], [62], hydronium (H₃O⁺) [33], [34], [63] and

hydrogen ion (H^+) [52], [53], [64] have been proposed. Each of these is strongly dependent on details of the assumed dissociation process. For instance, one of the possible electrochemical reactions is proposed in Fig. 2.4.

Figure 2.4: Schematic two-dimensional representation of the Si-SiO₂ interface, showing (a) the $\equiv SiH$ defect, (b) how this defect may be electrically activated during NBTI to form an interface trap, a fixed oxide charge, and a hydroxyl group, and (c) the OH diffuses through the oxide. [Extracted from Ref 31].

For a stable interface trap to be formed, the dissociated hydrogen species (e.g. a hydroxyl group like OH would be the diffusion species as illustrated in Fig. 2.4) have to be diffused away from the interface. When the concentration of the released hydrogen species decreases due to the diffusion, the reactions tend to favor the generation of interface states and/or the oxide charges accordingly. Some of the released hydrogen species can re-passivate the interface trap to form Si-H bond. Therefore, the essence of the diffusion-reaction model is that the rate at which the reaction causing the generation of interfacial defects take place is controlled by the diffusion of hydrogen that has been released from the hydrogen-passivated defect sites previously.

2.1.4 Effect of various process conditions on NBTI

NBTI is very sensitive to the processing conditions. A very comprehensive review on processing condition on NBTI can be found in Ref. 51. Here, we briefly discuss some of the key processing conditions that impact NBTI.

Hydrogen- As mentioned in previous section, hydrogen plays critical role in NBTI. It is a common impurity in MOSFETs, being incorporated into the oxide during various phase of IC fabrication, e.g. nitride deposition and forming gas annealing. Hydrogen has been found at concentration of 10^{19} cm^{-3} in dry oxides and concentration of 10^{20} cm^{-3} in wet oxides [65]. The distribution of hydrogen in oxides is non-uniform with a substantial pileup near SiO_2/Si interface [66]. Figure 2.5 depicts compares the H_2 and D_2 PMA on NBTI-induced threshold voltage shift. Evidently, hydrogen is involved in NBTI.

Figure 2.5: The effect of post metallization anneal ambient on the NBTI-induced ΔV_{th} .

Deuterium PMA suppress NBTI. [Re-plotted using data from Ref. 54].

Water- Water in the oxide enhances NBTI. Water or moisture can be incorporated through various oxidation ambients. For instance, “dry” oxide is grown in O_2 ambient, “damp” oxide is grown by exposing the dry oxide to a post metal annealing at 450°C , driving the water element to the Si/SiO₂ interface and “wet” oxide is grown in water vapor ambient. Blat *et al.* [33] carried out NBTI experiment using such dry, damp and wet oxides and observed that D_{it} and N_{ox} generation in damp and wet oxides whereas none in dry oxide. They concluded that water and hole must be present near the interface in order to observe NBTI degradations. Similar observation is also obtained from Ref. 54 and their result is shown in Fig. 2.6. The NBTI reaction is in the form

where A is water species and B^+ is dissociated hydrogen species. Helms *et al.* proposed that water as the NBTI culprit and in this situation H_2O is the most likely de-passivating reactant for Si-H bonds [34].

Figure 2.6: The effect of oxidation atmosphere on the V_{th} shift. Wet oxidation enhances NBTI. [Re-plotted using data from Ref. 54].

Boron- The effect of boron on NBTI is still controversial. Boron can diffuse into the gate oxide from the boron-doped gate. Figure 2.7 shows the comparison of NBTI-induced interface trap density and threshold voltage shift for pMOSFET with and without boron penetration. It can be seen that boron penetration can suppress the NBTI-induced interface trap generation. Indeed, boron penetration has been observed by Yamamoto *et al.* [37] to enhance positive oxide charge generation but to suppress interface trap generation. Reduced interface trap generation is attributed to formation of Si-F bonds from BF_2 boron implant [37], [67]. Enhanced positive oxide charge has been attributed to increased oxide defects due to boron in the oxides. Though reduced interface trap is observed, boron penetration generally degrades the NBTI lifetime of a pMOSFET [37].

Figure 2.7: BT stress time dependence of ΔN_{it} and ΔV_{th} for pMOSFET's with and without boron penetration. [Re-plotted using data from Ref. 37].

On the contrary, using different source/drain annealing temperatures to examine the effect of boron penetration in NBTI, Makabe *et al.* obtained opposite result [68]. Their result is shown in Fig. 2.8. They observed NBTI is suppressed with higher annealing temperatures and proposed that electron current from the gate electrode causes impact ionization at the SiO₂/Si interface. The generated holes jump into oxide due to the negative bias at gate electrode and some of them are trapped inside the oxide and cause NBTI degradations. Higher annealing temperatures cause more boron to be incorporated into the oxide, where it raises the barrier height and reduces the electron current from the gate electrode. This is the reason that higher annealing temperatures reduce NBTI degradation. More studies are thus needed to elucidate the role of boron in NBTI.

Figure 2.8: NBTI-induced ΔV_{th} dependence on S/D anneal temperature. $T_{ox} = 2.6$ nm; W/L is 10/10 μm ; BT stress voltage = -2.4 V and stress time 1000s. Higher annealing temperature shows smaller BT degradation. [Re-plotted using data from Ref. 68].

Fluorine- Fluorine reduces NBTI. Hook *et al.* reported that fluorine reduces NBTI and the reduction increases with increasing implanted fluorine dose [69]. Liu *et al.*, also observed an NBTI improvement [70]. The improvement can be attributed to the strong Si-F bond forming at the Si/SiO₂ interface, which increases the resistance against NBTI as compared to conventional Si-H bond.

Figure 2.9: ΔV_{th} versus stress time under NBTI stress for samples with or without F added to the 3.3-nm thermal oxide. [Re-plotted using data from Ref. 70].

Nitrogen- Nitrogen enhances NBTI. Nitrogen is commonly incorporated in gate oxide to suppress boron penetration issue, improve hot carrier resistant, and increase the dielectric constant. However, nitrogen is found to degrade NBTI [54], [70], [71] which we termed it as nitrogen-worsen NBTI effect. This is evidently shown in Fig. 2.10, which compares the NBTI-induced threshold voltage shift for pure and nitrated oxides. This observation is disturbing as gate oxide is further scaled; higher amount of nitrogen is required to suppress the boron penetration. However, the effect of nitrogen is only practically understood, more studies are necessary in order to understand the role of nitrogen in NBTI.

Figure 2.10: V_{th} shift due to NBTI for pure and nitrated oxide. A large V_{th} shift was observed for nitrated oxide. [Re-plotted using data from Ref. 54].

Interconnect- Figure 2.11 depicts the comparison of NBTI-induced ΔI_{d_sat} Cu/Low-k and Al/SiO₂ interconnect structure. It is apparent that NBTI lifetime of copper/low k interconnects is shorter than that of aluminium/SiO₂ interconnects [72]. The increased sensitivity of NBTI to copper metallization was attributed to increased hydrogen present in both the copper metallization and especially in the barrier metal.

Figure 2.11: Change in I_{d_sat} for pMOSFETs with different interconnect structures. [Re-plotted using data from Ref. 72].

In addition, comparison of NBTI performance for cap layers and inter metal dielectric (IMD) layers is shown in Fig. 2.12(a). From this result, it can be concluded that Si-C cap layer has higher NBTI immunity than that of Si-N cap layer as it is found that Si-C is permeable to water hence water can be desorbed to upper layer easily. On the contrary, Si-N is impermeable to water, so the water tends to diffuse to gate oxide and subsequently worsen NBTI [72]. Another area of significant importance with regard to

NBTI and backend-of-line (BEOL) is intermetal dielectric (IMD) [72], [73]. It can be observed from Fig. 2.12(a) that an organic low-k material (SiLK) has better NBTI performance as compared to PE-CVD SiO₂ [72]. This is attributed to less water in SiLK film than that in PE-CVD SiO₂. The final area of BEOL processing to impact NBTI performance is device antenna ratio and the potential for plasma damage [73]-[76]. Figure 2.12(b) shows a comparison of NBTI-induced ΔV_{th} of a control and antenna device. It is clear that plasma damaged devices (antenna device) become more sensitive to NBTI degradation with highly accelerated ΔV_{th} in comparison to diode-protected structures or structures without antennas connected. This is attributed to that higher number of Si-H bonds that are more likely to exist in plasma damaged devices [74], [77]. It has also been demonstrated recently that use of a thin conductive top films on top of the contact etch stop layer over silicon results in significantly reduced plasma damage and significant improvement in NBTI lifetime [76].

Figure 2.12: (a) Dependence of the $\Delta I_{d,sat}$ induced by NBTI stress on the cap layer (P-SiN, P-SiC) and IMD film (SiLKTM, P-SiO) [re-plotted using data from Ref. 72] and (b) ΔV_{th} vs. time for diode-protected (Control) and 120 K μ m (antenna device) under NBTI stress.. [Re-plotted using data from Ref 74].

2.2 Theory of atomistic modeling

The vast array of atomic scale simulation methods can be classified into two main categories depending on how they model physical phenomena in the simulated system: Classical and Quantum Mechanical (QM). We shall review some approaches adopted by each categories and explain the choice of method for our calculation.

2.2.1 Classical models

Classical model are often associated with Molecular Dynamic (MD). It uses the laws of classical physics to predict the structure and properties of molecules. MD calculations do not explicitly take into account the role of electrons in a molecular system. Instead, they perform computations based upon the interaction among the nuclei. The interaction energy is expressed by an interatomic potential energy function whose form is often derived empirically and thus makes use of fitted parameters. This approximation makes MD computations quite inexpensive, and allows them to be used for very large systems containing many thousands of atoms. Representative examples include the modeling of point defect diffusion and ion implantation damage [78], [79]. However, it also carries several limitations as well. Among the important are these:

- 1). Each interatomic potential energy function achieves good results only for a limited class of molecules, related to those for which it was parameterized. However, no potential energy function can be generally used for all molecular systems of interest. In addition, the extensive parameter fitting required to formulate an empirical potential is costly and time-consuming.

2). Neglect of electrons means that MD methods cannot treat electrochemical problems where electronic effects predominate. For example, they cannot describe processes, which involve bond formation or bond breaking. Molecular properties like band gap, which depend on subtle electronics details, are also not reproducible by MD methods.

Based on the limitation imposed on MD methods, they are not suitable to be used in developing the atomic model of NBTI, which generally involve bond dissociation during stress. Therefore, our choice of atomistic model has left with Quantum Mechanical models and we shall now briefly review some theories related to Quantum Mechanical.

2.2.2 Quantum mechanical models

Quantum mechanic explains how entities like electrons have both particle-like and wave-like characteristics. Quantum theory has also proven correct and provided fundamental understanding for a wide variety of phenomenon, including the energy levels of atoms, the covalent bond, and the distinction between metals and insulators [80]. Quantum theory is based on Schrodinger's equation in which electron are considered as wave-like particles whose "waviness" is mathematically represented by a set of wavefunctions obtained by solving Schrodinger's equation. The Schrodinger's equation of a particle is given by

$$\left\{ \frac{-h^2}{8\pi^2m} \nabla^2 + V \right\} \Psi(r,t) = \frac{ih}{2\pi} \frac{\partial \Psi(r,t)}{\partial t} \quad (2.8)$$

In this equation, Ψ is the wavefunction, m is the mass of the particle, h is Planck's constant, r is spatial position vector, t is time factor and V is the potential field in which the particle is moving. The product of Ψ with its complex conjugate is interpreted as the

probability distribution of the particle. If V is not a function of time, the Schrodinger equation can be simplified becomes the time-independent Schrodinger equation

$$\hat{H} \Psi(r) = E \Psi(r) \quad (2.9)$$

where E denotes the energy of either the ground or an excited state of the particle, and $\hat{H}$ is the *Hamiltonian operator*, equal to

$$\hat{H} = \frac{-\hbar^2}{8\pi^2 m} \nabla^2 + V \quad (2.10)$$

where the first term at the right hand side corresponds to kinetic energy and V corresponds to potential energy of the particle. The various solutions to Eq. (2.3) correspond to different stationary states of the particle. The one with the lowest energy is called the *ground state*. Equation (2.3) is a non-relativistic description of the system, which is not valid when the velocities of particles approach the speed of light. Thus, Eq. (2.3) does not give an accurate description of the core-electrons in large nuclei.

Most physical problems of interest consist of a number of interacting electrons and nuclei. The time independent many-body Schrodinger equation is then formulated as

$$\hat{H}(r_1, \dots, r_N) \Psi(r_1, \dots, r_N) = E \Psi(r_1, \dots, r_N) \quad (2.11)$$

where the Hamiltonian of the system is given by

$$\hat{H}(r_1, \dots, r_N) = \sum_{i=1}^N \frac{-\hbar^2}{8\pi^2 m_i} \nabla_i^2 + V^{nucl} + V^{elec} + V^{nucl-elec} \quad (2.12)$$

where N is the number of particles (electrons and nucleus) with position vectors r , E is the total energy of the system and V^{nucl} , V^{elec} , and $V^{nucl-elec}$ denote the potential energy arising from nuclei-nuclei repulsion, nuclei-electron attraction, and electron-electron repulsion, respectively. The total number of particles is usually sufficiently large that an exact solution cannot be found. Controlled and well-understood approximations are sought to

reduce the complexity to a tractable level. Once the equations are solved, a large number of properties may be calculated from the wavefunction.

The Born-Oppenheimer approximation is the first of several approximation used to simplify the solution of the many-body Schrodinger equation. It solves the general molecular problem by separating nuclear and electronics motions. This approximation is reasonable since the mass of a nucleus is thousands of times greater than that of an electron. The nuclei move every slowly with respect to the electrons, and the electrons react essentially instantaneously to the changes in nuclear position. Thus, the electron distribution within a molecular system depends on the positions of the nuclei, and not on their velocities. In other words, the nuclei look fixed to the electrons, and electronic motion can be described as occurring in a field of fixed nuclei. The full *Hamiltonian* for the molecular system can then be written as:

$$\hat{H} = T^{elec}(\vec{r}) + T^{nucl}(\vec{R}) + V^{nucl-elec}(\vec{R}, \vec{r}) + V^{elec}(\vec{r}) + V^{nucl}(\vec{R}) \quad (2.13)$$

where $\vec{r}$ are the electronic coordinates, $\vec{R}$ are the nuclear coordinates, T and V denote the kinetic and potential energy of the particles (nuclei or electron), respectively. This separation of the *Hamiltonian* into a sum of nuclear and electronic parts the separation of the Schrodinger equation and solved independently. So, one can construct an electronic *Hamiltonian* which neglects the kinetic energy term for the nuclei as their position fixed in space:

$$\hat{H}^{elec} = T^{elec}(\vec{r}) + V^{nucl-elec}(\vec{R}, \vec{r}) + V^{elec}(\vec{r}) + V^{nucl}(\vec{R}) \quad (2.14)$$

This $\hat{H}^{elec}$ is then used in the Schrodinger equation describing the motion of electrons in the field of fixed nuclei:

$$\hat{H}^{elec}\Psi^{elec}(\vec{r}, \vec{R}) = E^{eff}(\vec{R})\Psi^{elec}(\vec{r}, \vec{R}) \quad (2.15)$$

Solving this equation for the electronic wavefunction will produce the effective nuclear potential function E^{eff} . It depends on the nuclear coordinates and describes the potential energy surface for the system. Electronic structure calculations like first-principles method aim to solve the electronic Schrodinger equation as a function of the nuclear coordinates.

2.2.2.1 First-principles Density Functional Method

As mentioned in earlier section the aim of first-principles or *ab initio* method is to find such solution to the many-electrons Schrodinger equation, i.e. Eq. (2.5), for the system being studied. One of the approaches under first-principles method is called Density Functional Theory (DFT) [81]-[84]. DFT deals with the ground state of a quantum-mechanical many-body systems of electrons. The motivation of DFT is that the ground state properties of a system can be described by considering the ground state charge density.

Hohenberg and Kohn [81] proved that the total energy of an electron gas (even in the present of a static external potential) is a unique functional of the electron density. The minimum value of the total-energy functional is the ground-state energy of system, and the density that yields this minimum value is the exact single-particle ground-state density. This gives rise to the name “Density Functional Theory”. While the Hohenberg-Kohn theorem shows it is possible to use the ground state density to calculate properties of the system, it does not provide a way of finding the ground state density. Kohn and Sham [82] then showed how it is possible, formally, to replace the many-electron problems by an exactly equivalent set of self-consistent one-electron equations. Following

on the work of Kohn and Sham, the approximate functional employed by current DFT methods partition the electronic energy into several terms:

$$E = E^T + E^V + E^J + E^{XC} \quad (2.16)$$

where E^T is the kinetic energy term (arising from the motion of the electrons), E^V includes term describing the potential energy of the nuclear-electron attraction and of the repulsion between pairs of nuclei, E^J is the electron-electron repulsion term, and E^{XC} is the exchange-correlation term and includes the remaining part of the electron-electron interactions. These remaining interactions are:

- 1). The exchange energy arising from the antisymmetry of the QM wavefunction.
and
- 2). Dynamic correlation in the motions of the individual electrons.

The simplest method of describing the exchange-correlation energy of an electronic system is to use the local-density approximation (LDA) proposed by Kohn and Sham [82]. Hence, E^{XC} is determined entirely by the electron density as an integral involving only the spin density and possibly their gradient. However, the exchange function of LDA was developed to reproduce the exchange energy of a uniform electron gas. By itself, however, it has weaknesses in describing molecular system. Therefore, Becke [85] and Lee-Yang-Parr [86] have introduced a gradient correction to improve exchange and correlation functional, respectively. This produces the well-known B3LYP functional pairs for exchange correlation functional, which is now widely used.

Both wavefunction and density functional methods aim to compute properties of interest without recourse to experimental data. Doing this requires finding the wavefunction. As this is generally unknown, it is usual to expand it in terms of a set of known functions called basis set. For isolated atoms and molecules like in our cases, the

wavefunction exponentially decays to zero at large distances. This implies that the basis functions used for these calculations should do likewise. The size of the basis set has a large bearing on the accuracy of the calculation. Large basis sets more accurately approximate the orbitals by imposing fewer restrictions on the locations of the electrons in space. This is because, from QM point of view, electrons have a finite probability of existing anywhere in space; this limit corresponds to the infinite basis set expansions.

In short, Quantum Theory has proven correct and provided fundamental understanding for a wide variety of phenomena, including the energy levels of atoms, the covalent bond, and the distinction between metals and insulators. Further, in every instance of its application to date, the equations of quantum mechanics have yet to be shown fail. That is, therefore, every reason to believe that an understanding of a great number of phenomenon can be achieved by continuing to solve these equations.

2.2.3 The choice of method for NBTI atomic modeling

As mentioned earlier, Classical model is not suitable in this project which generally involve bond breaking like interface state generation. Furthermore, parameterization is needed in Classical model and shall be a very painstaking task. Another major drawback is the approach of solving Classical model is not as accurate as that of first-principles method. Therefore, only choice we have is first-principles density functional theory.

Almost every physically observable quantity is related to the total energy of a system or to differences in the total energy. The utility of atomic scale calculations lies in their ability to calculate the total energy of a system based on the microscopic arrangement of atoms and electrons within the material. For the understanding of NBTI

electrochemical reaction, the total energy approach enables the determination of quantities such as defect creation energies, reaction energies, and activation barriers. If quantum mechanical models are used, properties related to the electronic structure, such as band structures, and defect energy levels, can also be computed.

The main drawback of first-principles density functional theory approach is its intense computational cost, which severely limits the size of the system and the basis set which can be simulated. The larger basis set and system would inevitably increase the cost and computational time exponentially. To improve the system size and computational time, a super-fast supercomputer is inevitably needed. Therefore, due to our limited resource, a compromise is required to balance both cost and accuracy. In this regard, the size of the system is limited to 10~30 atoms.

Our theoretical approach is based on first-principle quantum chemistry calculations using the GAUSSIAN 98 suite [87]. We use the B3LYP hybrid gradient-corrected density functional function (DFT) method with Becke's exchange functional [85] and the Lee-Yang-Parr [86] correlation for all the electronic structure calculations. In our calculations, we adopted *Split valence basis set* with polarization function for all atoms. This allows molecular orbital to change size and shape hence give rise to reasonably accurate total energy calculations and computational time. The basis function is termed as 6-31g(*d*) and developed by Petersson and co-workers [88], [89]. The choice of the basis set is relied on whether it can adequately describe Hydrogen, Oxygen, Nitrogen and Silicon atom, which reside in pure and nitrided oxides. Indeed, It has been demonstrated 6-31g(*d*) can be used to describe the atoms from first-row till third row of periodic table [88]-[91]. Thus, B3LYP with 6-31g(*d*) will be used in this research work to calculate the total energy of various models related to pure and nitrided oxides.

2.2.4 First-principles density functional calculation procedure

2.2.4.1 Geometry optimization calculations

Geometry calculation is used to find the minima on the potential energy surface, with these minimization energy structures representing equilibrium structures. The procedure calculates the wave function and energy (solving the Schrodinger's equation presented in earlier session) at a starting geometry and proceeds to move to a new geometry, which will give a lower energy. This is then repeated until we have the lowest energy geometry close to the starting point. Ideally this procedure calculates the forces on the atoms by evaluating the gradient (first derivative) of the energy with respect to the atomic coordinates analytically. In some cases the gradients have to be estimated numerically. Sophisticated algorithms are used to select a new geometry at each step, which gives rapid convergence to the geometry with the lowest energy.

It is important to recognize that this procedure will not necessarily find the geometry of lowest energy, that is the lowest energy isomer or global minimum. It may find a local minimum, that of another isomer. It is a complex job to find all the isomers of a particular set of atoms. The optimization procedure actually finds a stationary point and this may be a transition structure or some other stationary point. We can sort out these problems by carrying out frequency analysis, which discuss in later part of this chapter.

It is always a good idea to do a geometry optimization with a small basis set and a lower method before we move to the basis set and method of choice for a particular problem. Therefore, we start a geometry optimization off from the geometry selected by Hartree-Fock with a basis set of 3-21g (small basis set and lower method) in all calculations involving pure and nitrided oxide. This will make the final run to optimize the geometry more efficiently.

2.2.4.2 Frequency calculations

We carry out frequency for two reasons. First, we may want to actually predict the frequencies, and Raman intensities. Here, we noted that the frequencies are harmonic frequencies-they are those obtained by assuming the potential energy surface is harmonic. However, we carry out frequency calculations much more often than this. If the geometry obtained from an optimization run is a local, or indeed the global, minimum, all the frequencies will be real and positive. Getting such a result confirms we have obtained a local or global minimum. If we have a transition structure or any satisfactory point other than a minimum, some of the frequencies will be complex. These are printed out as negative numbers and are often called “imaginary frequencies”. A well-behaved transition structure for a reaction will have one imaginary frequency. Note that frequency calculations should only be carried out at the geometry obtained from an optimization run and with the same basis set and method. Any other calculation will give meaningless results.

2.2.4.3 Atomic charge density calculations

As discussed earlier, NBTI can be described by a general electrochemical reaction. To provide further insight on NBTI, a set of atomic charges is needed for all molecules of interest. Unfortunately, such charges are not observable and hence they cannot be measured or calculated. Therefore a large number of methods have been suggested for their determination [92], e.g. Mulliken analysis [93], Nature population analysis [94], atoms in molecules [95], and electrostatic potential (ESP) derived charges [96]-[99].

It should be noted that the atomic charges vary widely between the different methods. This is mainly due to that the methods sample potential point differently (e.g. they use different inner and outer exclusion radii). Hence, there is no clear criterion for the quality of the charges. This is probably the reason why so many charge models have been suggested and unfortunately, no charge model is best in all respects. For example, topological methods give the best chemical properties, whereas the potential-based charges exhibit the best electrostatic properties. Since our aim is to obtain a relative comparison for the atomic charge of various atoms of interest, the quality of charges is beyond the scope of our study.

In our calculation, we compute the atomic charge density using Mulliken population analysis [93], Weinhold-Reed Natural Population Analysis (NPA) [94] and CHELP [96]. The first two are based on the molecular orbitals while in the third one are derived by fitting the electrostatic potential. Mulliken population analysis computes charges by dividing orbital overlap evenly between the two atoms involved. Nature Population analysis is carried out in terms of localized electron-pair “bonding” units. Its more detailed analysis also includes the number of core electrons, valence electrons and Rydberg electrons, located in diffuse orbitals. It also partitions the charge on each atom among the atomic orbitals. On the other hand, electrostatic potential-derived charge (CHELP) assigns point charges to fit the computed electrostatic potential at a number of points on or near the van der Waals surface.

2.3 Chapter summary

In this chapter, some prevailing NBTI models on pure SiO_2 are reviewed. Among them, the most widely accepted model would be diffusion-control electrochemical model. This is because they can offer satisfactory explanation for most of the experimental findings. The effect of processing conditions on NBTI is reviewed as well. However, most of these effects especially nitrogen are only practically understood, in-depth studies are necessary to elucidate the role of individual process. Following by that, a review of atomic scale modeling theory is also presented. The characteristics e.g. approach of solving equation and theory of the two main category of atomic modeling is discussed. Their advantages and drawbacks of each category are also made known. Based on the requirements for modeling NBTI reactions, first-principles-density functional theory is identified as the most promising method for the properties of interest though it still suffers from intense computational cost.

CHAPTER THREE

Dependence of NBTI degradation on nitrogen concentration at Si/SiO_xN_y interface

In this chapter, we present a comprehensive and quantitative study on the influence of nitrogen at the Si/SiO_xN_y interface on NBTI. In particular, with the pure SiO₂ as the control sample, the impact of nitrogen on time dependence, oxide field dependence and temperature dependence has been studied in detail. Detailed analysis of nitrogen effect on various stressing conditions leads to several conclusions that give us a better understanding of the role of nitrogen in NBTI. In addition, some correlation studies have been presented to offer better insight into the interactions of device degradation parameters. Consequently, several quantitative relationships between the interfacial nitrogen concentration and key parameters like NBTI thermal activation energy, interface trap and positive oxide charge density are obtained. A discussion on the mechanism of the nitrogen effect on oxide charge trapping and interface trap generation is also presented.

3.1 Introduction

Figure 3.1: The transition of lifetime limitation mechanism from HCI limited regime to BTI limited regime as a function of gate oxide thickness. The closed symbol denotes the V_{DD} voltage as predicted from SIA Roadmap, whereas the open symbol denotes the critical voltage V_{crit} between the two degradation mechanisms. For $V_{DD} > V_{crit}$, HCI degradation in n-MOSFET limits the CMOS lifetime whereas as $V_{DD} < V_{crit}$, BTI degradation in p-MOSFET limits the lifetime. [Re-plotted using data from Ref. 14].

As shown in Fig. 3.1, degradation of pMOSFET due to negative bias temperature instability (NBTI) is becoming an increasingly important reliability concern in processes under development and production in recent years [14], [54], [71], [100]. This stress occurs in both digital [100] and in analog [71] complementary MOS (CMOS), when devices are operated at elevated temperature with negative gate voltage. The BTI stress can shift the threshold voltage (ΔV_{th}) of a p-MOSFET by as much as 50 – 100 mV, due to

the creation of interface traps (N_{it}) and the buildup of positive oxide charges (N_{ox}) in the oxides over a period of months to years depending on the operating condition of the chip [14]. As a consequence, it would be more difficult to turn on pMOSFETs, causing a significant reduction in circuit speed. It has been reported that when oxide thickness is less than 3.5 nm, the threshold voltage shift of pMOSFET due to NBTI begins to limit the device lifetime [14]. Furthermore, several studies on the impact of gate oxide nitridation on NBTI have been reported and it is found that NBTI is exacerbated by the incorporation of excessive nitrogen into a gate oxide [54], [101]. Conversely, the effects of the replacement of hydrogen anneal by deuterium [54] or fluorine [101] anneal have also been reported for silicon dioxide film, showing the importance of interfacial Si-H bonds in NBTI degradation process. Although it is known that holes and hydrogen are involved in the degradation process, the role of nitrogen has not been sufficiently discussed. In particular, recent studies on the nitrogen effect are restricted to process-condition dependence rather than nitrogen concentration dependence. Incorporation of nitrogen into gate oxide is still under investigation because its effect is only practically understood empirically. Furthermore, as gate oxide with higher nitrogen content will be used in future-generation MOS devices; NBTI will be a critical degradation issue.

3.2 Device fabrication and NBTI experimental setup

Devices were fabricated using 0.13 μm CMOS technology on 200 mm *p*-type Si substrate. After the formation of retrograde well and shallow trench isolation, gate oxides with thicknesses T_{ox} ranging from 1.8 to 6.5 nm were grown by rapid thermal oxidation. The oxides were then exposed to *in-situ* rapid thermal nitridation in an NO gas ambient. To study the role of nitrogen, various nitrogen concentrations were achieved at different

nitridation temperatures/durations/pressures. Upon nitridation, all the samples received identical post-nitridation annealing. Subsequently, 160 nm un-doped polysilicon was deposited and patterned. The gate electrodes and source/drain were doped simultaneously by boron implantation, followed by dopant activation using rapid thermal spike annealing. Finally, after formation of interconnects metal layer, sintering was accomplished in a forming gas ambient. Unless otherwise specified, transistor used in this research work has a width (W) and length (L) of 10 μm and 0.12 μm respectively, and a T_{ox} of 1.8 nm.

Figure 3.2: Depth profiles of nitrogen as determined from secondary ion mass spectroscopy (SIMS), for various nitridation conditions as shown in the inset.

The nitrogen depth profiles of the nitrided oxides were determined using secondary ion mass spectroscopy as shown in Fig. 3.2. It is consistent with previous studies [102] that thermal nitridation generally results in a sharp nitrogen peak at the interface. Samples with four interfacial nitrogen concentrations N_{int} (2.8, 4.5, 5.5, and 7.5 at. %) were used in this study. The gate oxide thickness T_{ox} of 1.8 nm was determined from high-resolution transmission electron microscopy (HRTEM) [inset of Fig. 3.2].

NBTI stress was applied, with the gate electrode of a p-MOSFET held at low constant negative bias, ranging from -2 to -3 V, under elevated temperature (100 – 150 °C). The S/D and substrate electrodes were grounded. The NBTI bias configuration is illustrated in Fig. 3.3(a). The stress was interrupted at pre-determined time to measure the V_{th} and G_m [at $V_d = -0.1$ V] at the same stress temperature. A typical ΔV_{th} measurement is shown in Fig. 3.3(b). An automated BTI test program written in QBASIC is used to perform the experiment to mitigate any error induced by time lapse between the measurements and stressing. The source code of the program is listed in Appendix A.

Figure 3.3: (a) Illustration of the NBTI bias configuration; (b) typical ΔV_{th} measurement.

To further characterize the NBTI, the amount of interface traps was monitored on a large area pMOSFET W/L= 100/10 $\mu\text{m}/\mu\text{m}$ using direct-current current-voltage (DCIV) [103], [104] method at room temperature. DCIV measurement is used here because the excessive direct-tunneling leakage current in our ultra-thin gate oxide samples renders the conventional methods, such as quasi-static C-V and charge-pumping methods, inappropriate for probing the interface states. From the measured DCIV I-V plots, the effective interface trap density (D_{it}) was calculated from the peak DCIV base current ($I_{b,peak}$) using the following formula [103]:

$$I_{b,peak} = \frac{qD_{it}An_i c_s}{2} (\exp(\frac{qV_{eb}}{2kT}) - 1) \quad (3.1)$$

where V_{eb} is the forward emitter bias, A is the device area, n_i is the intrinsic carrier concentration, q is the electronic charge, T is the measurement temperature, and c_s is the capture cross-section.

Figure 3.4: Correlation study between the DCIV method and subthreshold swing change on NBTI-induced D_{it} .

For pMOSFET with W/L= 10/0.12 $\mu\text{m}/\mu\text{m}$, subthreshold swing change [105] was used to monitor the D_{it} generation at the stress temperature instead of the DCIV method. This is because for devices with small area, DCIV technique is inadequate to capture the DCIV current due to the small signal-to-noise ratio. Figure 3.4 depicts a correlation study between DCIV method and subthreshold swing change on NBTI-induced interface trap generation. Both methods have been performed on the same large structure, which underwent NBTI stress. A linear correlation between the two methods validates the subthreshold swing method used for interface trap density in small area device.

Conversely, the oxide charges (N_{ox}), which are the charges in the oxide near the Si/SiO₂ interface, contribute to the ΔV_{th} as well. Measurement of midgap voltage shift (ΔV_{MG}) has been widely used to monitor the generation of N_{ox} , [31],[32],[35],[105]. It is based on the general assumption that interface traps are in the upper half of the band gap are acceptors and those in the lower half of the band gap are donors, having interface traps uncharged at the midgap condition ($\phi_s = \phi_F$). First, the midgap current I_{MG} , defined as the current at the midgap condition, is obtained from the subthreshold current equation

$$I_D = \mu_{eff} \left(\frac{W}{L} \right) \frac{aC_{ox}}{2\beta^2} \left(\frac{n_i}{N_A} \right) (1 - e^{-\beta V_d}) (e^{-\beta \phi_s}) (\beta \phi_s)^{-1/2} \quad (3.2)$$

where μ_{eff} is the effective mobility, $\beta = q/kT$, and n_i is the intrinsic carrier concentration. Solving Eq. (3.2), one obtains the I_{MG} . After that, the experimental subthreshold curve at the stress temperature is linearly extrapolated to the I_{MG} to locate the V_{MG} [105] and, thus, the corresponding ΔV_{MG} can be monitored with stress. Finally, effective density of the oxide charges (ΔN_{ox}) located at the interface can be found from the measured ΔV_{MG} as $\Delta N_{ox} = (C_{ox} \Delta V_{MG}) / q$. In this case, C_{ox} is the MOS capacitance per unit area.

3.3 Results

3.3.1 Nitrogen effect on the time dependence of threshold voltage shift

Figure 3.5 shows the threshold voltage shift ΔV_{th} as a function of stress time, for p-MOSFET with various interfacial nitrogen concentrations (N_{int}). For comparison, ΔV_{th} of the control sample (i.e. pure SiO₂) is also included. As can be seen from the figure, regardless of N_{int} , a power-law relationship exists between ΔV_{th} and stress time t :

$$\Delta V_{th} = At^n \quad (3.3)$$

where the prefactor A is dependent of the nitrogen concentration, while the exponent factor n (ranging from 0.20 to 0.22) shows negligible dependence on the nitrogen

Figure 3.5: Typical threshold voltage shift (ΔV_{th}) as a function of NBTI stress time for p-MOSFET with various interfacial nitrogen concentrations (N_{int}). For comparison, ΔV_{th} of the control sample (i.e. pure SiO₂) is included.

concentration. This is consistent with previous studies, in which the time exponent factor was found to be independent of the interfacial nitrogen concentration [54], [101]. It has been shown that $n \leq 0.25$ is related to a diffusion-controlled electrochemical reaction [31], [35], [50]. Since the observed n values here are smaller than 0.25, it is thus suggested that the NBTI degradation for both pure- and nitrided oxide is governed by diffusion-limited reactions where the diffusion of reaction species, such as hydrogen-related species, is the dominating mechanism in the NBTI. On the other hand, it has been reported that the prefactor A is a product of thermal activation energy E_a and oxide field E_{ox} [17], [74]. The dependence of A on the N_{int} implies that nitrogen has an effect on either the thermal activation energy or the oxide field, or the initial concentration of defects. We shall clarify this issue in the following sections.

3.3.2 Nitrogen effect on oxide field dependence of the threshold voltage shift

Figure 3.6 depicts the time dependence ΔV_{th} for various NBTI stress voltages. Using a power-law fitting, it is found that prefactor A depends largely on stress voltage, being consistent with reported literatures [54], [74]. However, exponent factor n (~ 0.21) is independent of stress voltage suggesting that the degradation mechanism is the same. To study the impact of nitrogen on the oxide field dependence of threshold voltage shift, we first compute the oxide field using

$$E_{ox} = \frac{V_g - V_{poly}}{T_{ox}} \quad (3.4)$$

where V_{poly} is the voltage drop in the poly-silicon gate due to band bending and can be calculated using

$$V_{poly} = \frac{\epsilon_{ox}^2 E_{ox}^2}{2q\epsilon_{si}N_p} \quad (3.5)$$

where N_p is gate doping concentration (cm⁻³), ϵ_{ox} and ϵ_{si} are permittivities of SiO₂ and Si, respectively.

Figure 3.6: ΔV_{th} as a function of stress time for various stress voltages. The line is fitted using power-law. The N_{int} of this work is 4.5 at. %.

Figure 3.7 shows the normalized ΔV_{th} as a function of oxide field for pure SiO₂ and SiO_xN_y with 2.8 and 4.5 at. %. Note that ΔV_{th} has been normalized to the time exponent factor. Based on this figure, it is obvious that oxide field enhances NBTI-induced ΔV_{th} . Being consistent with previous studies [31], [33], [58], the normalized ΔV_{th} follows an exponential relationship with oxide field, as given by

$$\Delta V_{th,normalized} = k \exp\left(\frac{E_{ox}}{E_1}\right) \quad (3.6)$$

where the prefactor k is a constant which depends on the initial concentration of surface defect N_D and thermal activation energy; whereas E_f is field accelerator factor which depends on process conditions. In this scenario, enhancement of ΔV_{th} with increasing oxide field could be due to the following reasons: (1) activation energy for hydrogen dissociation of the Si-H bonds is reduced as the free carrier density increases [57], (2) higher oxide field enhances the drift of the dissociated hydrogen ions and the electrochemical reactions. More importantly, nitrogen has a negligible impact on the accelerator factor E_f , which is approximately equal to 2.25 MV/cm. In contrast, the prefactor constant k is found to be 2.70×10^{-5} , 3.52×10^{-5} , and 5.63×10^{-5} V/sⁿ, for pure SiO₂, and nitrided oxides with interfacial N concentrations of 2.8 at. % and 4.5 at. %, respectively. The prefactor k increases with nitrogen concentration suggesting that the thermal activation energy decreases with increasing nitrogen content.

Figure 3.7: ΔV_{th} as a function of oxide field for various N_{int} .

3.3.3 Nitrogen effect on temperature dependence of the threshold voltage shift

To further probe the influence of nitrogen, we have investigated the temperature dependence of the nitrogen-worsen NBTI effect. Figure 3.8 shows the Arrhenius plots of the threshold voltage shift for the pure oxide and the two nitrided oxides with different N_{int} , after an NBTI stress at $V_g = -2$ V for 1000 s. As can be seen in Fig.3.8, the pure oxide exhibits stronger temperature dependence as compared to the nitrided oxides, and the temperature dependence is weaker for higher N_{int} . The thermal activation energies (E_a) extracted from the slope of the Arrhenius plots are 0.24, 0.18, and 0.14 eV for the pure oxide and the nitrided oxides with $N_{int} = 4.5$ and 5.5 at. %, respectively.

Figure 3.8: Arrhenius plots of ΔV_{th} for the pure oxide and nitrided samples (i.e. 4.5 and 5.5 at. %), $W/L = 100/10$ $\mu\text{m}/\mu\text{m}$.

More will be discussed on the observed dependence of E_a on N_{int} in the later section. The decrease in the activation energy with nitrogen concentration can be translated to a severe reduction in the NBTI lifetime for nitrided oxides although the degradation remains proportional to $t^{0.20}$ for both pure- and nitrided oxides. This result poses a serious reliability alarm for future technology, as higher nitrogen dose is needed to suppress the boron penetration.

3.3.4 Correlation study of threshold voltage shift with transistor performance

Figure 3.9: Correlation study between degradation of ΔI_{ds} and ΔV_{th} for various N_{int} . I_{ds} is measured at $V_g = V_d = -1.2$ V.

To examine the correlation between ΔV_{th} and transistor performance, Figure 3.9 shows a correlation study between the degradation of drain current and ΔV_{th} . A perfect

linear correlation is found and this relationship is independent of N_{int} . This indicates an increase of threshold voltage proportional to drain current reduction with a slope of 6.5 mA/V. In addition, the degradation of I_{dsat} and V_{th} in both pure SiO₂ and nitrided oxides are probably due to the same origin of defects generation. Therefore, no matter the degradations are due to nitrogen-related defects or hydrogen-related defects, both share common characteristics of degradation. In addition, further correlation study showed in Fig. 3.10 reveals yet other linear relationships of (a) ΔV_{th} and midgap voltage shift ΔV_{MG} and (b) ΔV_{th} and transconductance shift ΔGm_{max} for various N_{int} .

Figure 3.10: Correlation study of (a) ΔV_{th} and midgap voltage shift ΔV_{MG} and (b) ΔV_{th} and ΔGm_{max} for various N_{int} .

Being consistent with Fig. 3.9, the correlation is independent of N_{int} . In general, ΔV_{MG} and ΔGm_{max} suggest the creation of positive oxide charge N_{ox} and interface trap N_{it} , respectively. Therefore, both N_{ox} and N_{it} could be the primary defects for both pure SiO₂ and nitrided oxides. Another interesting observation found from Fig. 3.10(a) shows that

ΔV_{MG} is approximately half of ΔV_{th} for both pure SiO₂ and nitrided oxides. This suggests that positive oxide charge generation is responsible for half of the total ΔV_{th} whereas interface trap generation accounts for another half. In other words, there should be an equal amount of N_{ox} and N_{it} generation in both pure SiO₂ and nitrided oxide. Furthermore, both N_{ox} and N_{it} should be proportionally increased with N_{int} in order to explain nitrogen-worsen ΔV_{th} observed in Fig. 3.5. Therefore, based on this result, it is believed that the one to one correlation between N_{ox} and N_{it} is valid in both pure oxide and nitrided oxides.

3.3.5 NBTI-induced positive oxide charge and interface trap generation in nitrided oxides

To further understand the defects responsible for the ΔV_{th} of nitrided oxides, the positive oxide charge trapping (ΔN_{ox}) and the interface state generation (ΔD_{it}) are measured by monitoring the mid gap voltage shift and the subthreshold swing change, respectively. Figure 3.11(a) shows ΔN_{ox} as a function of stress time for various N_{int} . It is evident that for all samples ΔN_{ox} follows a power-law dependence on the stress time given as below

$$\Delta N_{ox} = Bt^n \quad (3.7)$$

where B is the prefactor governed by N_{int} , and t is the stress time. The exponent factor n (~ 0.25) is almost independent of N_{int} , being consistent with the stress-time dependence of ΔV_{th} shown in Fig. 3.5. This again indicates that both pure oxide and nitrided-oxides have similar degradation mechanism. To study nitrogen concentration quantitatively, ΔN_{ox} after 1000 s NBTI stress is obtained as a function of N_{int} , as shown in Fig. 3.11(b) to illustrate the nitrogen dependence. It is found that ΔN_{ox} has a linear dependence on N_{int}

with the following quantitative relationship

$$\Delta N_{ox} = 4.88 \times 10^{10} [0.48 N_{int} + 1] \quad (3.8)$$

where ΔN_{ox} is in cm⁻² and N_{int} is in at. %. This figure clearly spells the nitrogen-worsen NBTI effect where nitrogen enhances the positive fixed charge generation. With the nitrogen-worsen NBTI effect taken into account, Eq. (3.7) can be rewritten as

$$\Delta N_{ox} = A_{N_f, SiO_2} t^n [B_{N_f} N_{int} + 1] \quad (3.9)$$

where $A_{N_f, SiO_2} = 8.68 \times 10^9 \text{ cm}^{-2} \text{ s}^{-1/4}$ is the pre-factor for N_{ox} generation in pure SiO₂ and $B_{N_{ox}} = 0.48 \text{ (at.\%)}^{-1}$ is the nitrogen enhancement factor for the N_{ox} generation.

Figure 3.12(a) shows ΔD_{it} as a function of stress time for various N_{int} . Similar to ΔN_{ox} , ΔD_{it} also has a power law dependence on stress time. Figure 3.12(b) shows the ΔD_{it} after 1000 s NBTI stress as a function of N_{int} , and the following quantitative relationship is found

$$\Delta D_{it} = 3.92 \times 10^{10} [0.39 N_{int} + 1] \quad (3.10)$$

Furthermore the time evolution of ΔD_{it} can be expressed as

$$\Delta D_{it} = A_{D_{it}, SiO_2} t^n [B_{D_{it}} N_{int} + 1] \quad (3.11)$$

where $A_{D_{it}, SiO_2} = 6.97 \text{ cm}^{-2} \text{ eV}^{-1} \text{ s}^{-1/4}$ is the pre-factor for the D_{it} generation in pure SiO₂ and $B_{D_{it}} = 0.39 \text{ (at.\%)}^{-1}$ is the nitrogen enhancement factor for the interface trap generation. Thus, it is clear that the nitrogen incorporation increases the interface trap generation.

The comparison among Figs. 3.5, 3.11(a) and 3.12(a) provides strong proof to the existence of a close link between defect generation (positive oxide charge trapping and interface trap generation) and the threshold voltage shift. Hence, it can be concluded that both positive oxide charge and interface trap are the primary defects responsible for threshold voltage shift.

Figure 3.11: (a) ΔN_{ox} as a function of stress time for various N_{int} . The NBTI stress was carried out at the $V_g = -2.2 \text{ V}$ under the temperature of 125°C . (b) ΔN_{ox} as a function of N_{int} . The ΔN_{ox} is obtained after 1000 s of NBTI stress at the conditions used in Fig. 3.11a.

Figure 3.12: (a) ΔD_{it} as a function of stress time for various N_{int} . The NBTI stress was carried out at $V_g = -2.2 \text{ V}$ under the temperature of 125°C . (b) ΔD_{it} as a function of N_{int} . The ΔD_{it} is obtained after 1000 s of NBTI stress at the conditions used in Fig. 3.12a.

Figure 3.13: Correlation of positive oxide charge and interface trap density for various nitrogen concentrations. The data are obtained from Figs 3.11 and 3.12.

In addition, as cited in Chapter Two, both positive oxide charge and interface trap density increase proportionally during NBTI stress for pure SiO₂. We observed that this unique feature remains unaffected in nitrided oxide as can be seen from the correlation study in Fig. 3.13. The trend is also evidently unaffected by increasing interfacial nitrogen concentration. Furthermore, based on the results shown in Fig. 3.10a and the correlation study shown in Fig. 3.13, it can be concluded that the ratio of N_{ox} to N_{it} is approximately equal to unity. It should be noted that as demonstrated in [58], the NBTI-induced surface trap distributes over an energy range of ~ 1 eV, and therefore D_{it} is almost equal to N_{it} .

3.3.6 Relationship between interfacial nitrogen concentration and E_a of

N_{ox} and N_{it} generation in nitrated oxide

It has been shown in Fig. 3.8 that nitrogen reduces the thermal activation energy of the threshold voltage shift. To shed more light on nitrogen-worsen NBTI effect, thermal activation energies for both charge trapping and the interface trap generation are studied. Figure 3.14 shows the comparison of the Arrhenius plots of the NBTI-induced positive oxide charge trapping (ΔN_{ox}) between the pure oxide and the nitrated oxide with $N_{int} = 2.8$ at. %. The E_a for the charge trapping extracted from the Arrhenius plots are 0.21 and 0.15 eV for the pure oxide and the nitrated oxide, respectively. Obviously, the nitrogen reduces the E_a and enhances the positive oxide charge-trapping rate that is proportional to $\exp(-E_a/kT)$. This is consistent with the N_{int} dependence of the ΔN_{ox} shown in Fig. 3.11, which clearly spells the nitrogen-worsen NBTI effect.

Figure 3.14: Arrhenius plots of ΔN_{ox} for the pure oxide and nitrated oxide with 2.8 at. %.

On the other hand, the NBTI-induced interface trap generation has been studied by using the DCIV method. Figure 3.15(a) shows the influence of the NBTI stress temperature on the DCIV characteristics for the nitrated oxide with $N_{int} = 2.8$ at. %. The DCIV current (I_{DCIV}) is formed by electron-hole recombination via the interface states [103], [104], and hence the peak ($I_{DCIV,peak}$) is proportional to interface trap density. Figure 3.15(a) indicates that there is a large increase in the $I_{DCIV, Peak}$ after NBTI stress and the $I_{DCIV, Peak}$ increases with the stress temperature. The interface trap density before and after stress can be obtained with Eq. 3.1, and thus the interface trap generation (ΔD_{it}) is determined. As examples, the Arrhenius plots of ΔD_{it} for the pure oxide and the nitrated oxide with $N_{int} = 2.8$ at. % are shown in Fig. 3.15(b). The E_a obtained from the Arrhenius plots are 0.21 and 0.16 eV for the pure oxide and the nitrated oxide, respectively. This clearly indicates that the nitrogen incorporation can also reduce the E_a for the interface trap generation similar to the situation of oxide charge trapping shown in Fig. 3.14.

To elucidate the nitrogen-worsen NBTI effect, the activation energies (E_a) for both the charge trapping and the interface trap generation have been obtained as a function of interfacial nitrogen concentration (N_{int}), as shown in Fig. 3.16. The E_a obtained for the interface trap generation in pure SiO₂ is 0.21 eV, which is consistent with the result reported by Ogawa *et al.* (In their work, the E_a of interface trap generation in pure SiO₂ was found to be 0.18–0.20 eV). As can be seen in Fig. 3.16, the pure oxide exhibits the largest E_a , and E_a decreases monotonically as more nitrogen is incorporated at the Si/SiO_xN_y interface. The charge trapping and the interface trap generation have the same E_a within the experimental errors for a given interfacial nitrogen concentration.

Figure 3.15: (a) DCIV characteristics before and after NBTI stress with different stress temperatures for nitrated sample with 2.8 at % of N_{int} . (b): Arrhenius plots of interface trap generation (ΔN_{it}) for the pure oxide and for nitrated sample with 2.8 at % of N_{int} .

Figure 3.16: Activation energies of both the fixed charge trapping and the interface trap generation as a function of interfacial nitrogen concentration.

In addition, as demonstrated in Fig. 3.16, their E_a are found to follow the identical dependence on the N_{int} , i.e.,

$$E_a = 0.213 - 0.016N_{int} \quad (3.12)$$

where E_a is in eV and N_{int} is in at.%. These results unambiguously suggest that the charge trapping and the interface state generation have the same origin.

3.4 Minimization of NBTI through plasma nitridation

Until this point, the discussion has focused on the impact of interfacial nitrogen concentration on NBTI degradation. The importance of keeping the nitrogen concentration low at the interface is emphasized in order to suppress NBTI. However, nitrogen incorporation is needed to circumvent boron penetration from the gate electrode and more nitrogen content is needed when gate oxide thickness is further scaled. Therefore, an optimization of fabrication process is needed and this lead to the emerging of nitrogen profile engineering. In theory, if one can shift the nitrogen peak profile away from the interface in order to reduce the interfacial nitrogen concentration yet maintain a high content of nitrogen at the bulk oxide; both boron penetration and NBTI might be minimized. Recently plasma nitridation has attracted considerable interest over NO nitridation for sub-90 nm CMOS technology because of its superior efficiency in tailoring a higher amount of nitrogen near the polysilicon/SiO₂ interface and reducing nitrogen content at the Si/SiO₂ interface. This nitrogen-rich layer not only increases the dielectric constant of a nitrided oxide, which is useful in reducing the tunneling leakage current, but also acts as an excellent barrier to suppress impurity penetration. Therefore, it would be of great interest to study the effect of plasma nitridation on NBTI and Si/SiO₂ interface properties.

3.4.1 Experimental

To study the effect of plasma nitridation on NBTI, pMOSFETs with plasma-nitrided oxides of 2.6 nm were used. The plasma-nitrided oxides were prepared by exposing the base oxides to an *ex-situ* high-density decoupled nitrogen plasma source at room temperature. These oxides shall be referred to as decoupled plasma-nitrided oxide

(DPNO) hereafter for brevity. For comparison, rapid thermal nitrided oxides (RTNO) with the same oxide thickness, which were formed by subjecting the base oxides to *in-situ* rapid thermal nitridation in a NO ambient, were also studied. Upon nitridation, both DPNO and RTNO received identical post-nitridation annealing. Note that a careful optimization on thermal budget is required to tailor the peak profile near the oxide surface for the DPNO. The nitrogen depth profiles for both the DPNO and the RTNO were determined by SIMS and shown in the inset of Fig. 3.17(b).

3.4.2 Comparison of interfacial quality between DPNO and RTNO

To compare the interfacial quality between DPNO and RTNO, Figs. 3.17(a) and 3.17(b) show the comparison of effective channel hole mobility (μ_{effp}) and charge pumping current (CP), respectively, for 2.6 nm thick RTNO and DPNO. As can be seen from Fig. 3.17(a), DPNO shows a higher μ_{effp} than RTNO for all electric fields. The mobility is obtained through split-CV method [106]. The peak mobility for RTNO is degraded by 7% as compared to DPNO. In addition, no significant alternation of the μ_{effp} behavior can be detected for DPNO with RTNO implying that their mobility scattering mechanism is the same. Previous studies have attributed the degradation of μ_{effp} in thermally nitrided oxides to additional Coulombic scattering from nitridation-induced positive fixed charges and charged donor-like interface traps, as well as the reduction of mobile hole density due to hole trapping at near interfacial traps [107]-[109]. This suggests that DPNO reduces such scattering centers partially as compared to RTNO.

Figure 3.17: Plots of charge pumping current as a function of gate pulse frequency for 2.6 nm thick RTNO and DPNO. The inset depicts SIMS nitrogen profile for RTNO and DPNO respectively and their peak nitrogen conc. is 3 at. %. The device W/L = 20/0.5 μm .

To make clear on the distinct μ_{effp} behavior of DPNO, interface trap densities for 2.6 nm thick RTNO and DPNO have been monitored using CP current measurement. The results are depicted in Fig. 3.17(b). The CP current shows a linear dependence with the gate pulse frequency, indicating that the tunneling current component is negligible as compared to the CP signal [110]. As shown in Fig. 3.17(b), the CP current for DPNO is found to be substantially smaller than that for RTNO, signifying a lower intrinsic interface-trap density D_{it} in DPNO. Comparing Figs. 3.17(a) and 3.17(b), it is interesting to note that the behavior of interface-trap density and μ_{effp} are in good agreement, indicating a plausible link between them. For RTNO, the nitrogen piles up mainly at the Si/SiO₂ interface as depicted in the inset of Fig. 3.17(b). Excessive nitrogen at the Si/SiO₂ interface can unduly compromise the interfacial quality. In contrast, the behavior of μ_{effp} and D_{it} density for DPNO can be accounted for by the fact that the nitrogen is distributed essentially near the top oxide surface, and thus is spatially removed from the Si/SiO₂ interface as depicted in the inset of Fig. 3.17(b). As a result, DPNO is less susceptible to nitridation-induced D_{it} generation, and accordingly smaller μ_{effp} degradation.

3.4.3 Impact of nitrogen profile on NBTI

3.4.3.1 Time dependence of NBTI-induced ΔV_{th} & ΔI_{Dsat} for DPNO and RTNO

Figure 3.18(a) and (b) show the comparison of the NBTI induced ΔV_{th} and NBTI-induced saturation drain current ΔI_{Dsat} , respectively, for time dependence for 2.6 nm thick RTNO and DPNO oxide. The time dependence of ΔV_{th} is subjected to stress voltage ranging from -2.6 to -4 V for RTNO and DPNO. It is evident that this ΔV_{th} obeys a power-law dependence on time. Additionally, the exponent value of the ΔV_{th} and the

Chapter 3: Dependence of NBTI degradation on nitrogen concentration at Si/SiO_xN_y interface

ΔI_{dsat} is found to be insensitive to the oxide field and nitridation process. This is consistent with the earlier findings in section 3.3.1. The exponent value of the ΔV_{th} is found to be 0.25 for RTNO and DPNO. This identical time exponent value indicates that the mechanism of NBTI is independent of the nitrogen profiles and stress voltages. More importantly, DPNO exhibits less susceptibility to NBTI for all stress voltage range as compared to RTNO despite that both oxides have comparable peak nitrogen concentrations. This is consistent with a recent study on remote plasma nitridation [70]. Careful comparisons between this result and section 3.3 shows a large similarity, and this emphasizes again the role of interfacial nitrogen in the nitrogen-worsen NBTI effect. The suppression of DPNO can be attributed to its ability to displace the nitrogen peak profile away from the Si/SiO_xN_y interface hence reducing the amount of nitrogen content at the interface. This is confirmed by the SIMS profile in Fig. 3.17(b), although both RTNO and DPNO have peak nitrogen concentration of 3 at. %, DPNO has better immunity against NBTI as compared to RTNO. This indicates that interfacial nitrogen plays a critical role during NBTI degradation whereas nitrogen at bulk oxide plays a trivial role.

Figure 3.18: Comparison of time dependence of (a) NBTI-induced ΔV_{th} and (b) NBTI-induced saturation drain current ΔI_{dsat} for 2.6 nm thick RTNO and DPNO.

3.4.3.2 Lifetime dependence on nitrogen profile

Figure 3.19 compares the NBTI lifetimes for (a) RTNO and DPNO and (b) 12 s and 120 s re-oxidized nitrided oxide. The NBTI lifetime is defined as the time required for a threshold voltage shift of 50 mV at 125 and 150 °C for Figs 3.19(a) and 3.19(b), respectively. With the ability of alleviating the undesirable nitrogen-worsen NBTI effect, the DPNO can prolong the device lifetime by one order of magnitude as compared to the RTNO as depicted in Fig. 3.19(a). Figure 3.19(b) compares the NBTI lifetime as a function of gate voltage between two sets of 2 nm thick RTNO with post-nitridation re-oxidation (PNRO) duration of 12 and 120 s, respectively. It is clear that NBTI lifetime improves with longer PNRO duration.

It is known that PNRO following RTNO process will displace the nitrogen peak away from the Si/SiO₂ interface without significantly altering the nitrogen density [111]. The nitrogen depth profiles for RTNO with 12 and 120 s of PNRO have been verified by SIMS measurements, as showed in the inset of Fig. 3.19(b). Hence, the results in Figs. 3.19(a) and 3.19(b) clearly indicate that the proximity of nitrogen from the Si/SiO₂ interface plays a crucial role in the nitrogen-worsen NBTI effect. This is likely to happen predominately at the Si/SiO₂ interface and the effect diminishes as the nitrogen is situated away from the Si/SiO₂ interface.

Figure 3.19: Lifetime comparison for (a) RTNO and DPNO and (b) 12 s and 120 s re-oxidized nitrided oxide.

3.5 Discussion

As cited previously, it has been shown that the stress-time (t) dependence of the interface trap generation or threshold voltage shift follows a fractional power-law with an exponent of 0.25 in pure SiO₂. The ubiquitous $t^{0.25}$ has been attributed to the following diffusion-limited electrochemical reactions

The interface trap ($Si_3\equiv Si\bullet$ or $O_3\equiv Si\bullet$) and positive oxide charges ($Si-OH^+-Si$) are generated from the dissociation of $Si-H$ bonds [$Si_3\equiv Si-H$ or $O_3\equiv Si-H$] by holes in the Si inversion layer during NBTI stress. Ogawa *et al.* suggested that the E_a is related to the diffusion of the dissociated hydrogen species in which net defects generation is determined by the concentration of hydrogen species [31], [35], [50]. In this scenario, the diffusion of the hydrogen species from the interface to the bulk of the SiO₂ favours the forward reactions of Eqs. (3.13) and (3.14), enhancing the speed of the reaction. During diffusion, hydrogen species get trapped by bridging $Si-O-Si$ bond, thus, forming positive oxide charge $Si-OH^+-Si$. Therefore, the reduction of the concentration of the dissociated hydrogen at the interface actually determines the interface trap generation and charge trapping at the interface. From this viewpoint, the nitrogen-worsen NBTI effect (i.e. the activation energy decreases linearly with interfacial nitrogen concentration) could be linked to the following two effects: 1) the incorporation of nitrogen enhances the trapping of the dissociated hydrogen species at the Si/SiO_xN_y interface; and 2) released hydrogen species can diffuse out from gate dielectric more easily for SiO_xN_y layer than that of SiO₂

layer. These effects, which lead to the reduction of the concentration of the dissociated hydrogen species at the interface, increase the reaction rates of the forward reactions depicted in Eqs. (3.13) and (3.14) and thus enhance the interface trap generation and oxide charge trapping.

On the other hand, it has long been understood that NBTI degradation involves many reactions like dissociation, diffusion, trapping and etc. Therefore, it is argued in [31] that the reaction rate constant R_1 for defects generation [$\Delta V_{th} = R_1 * t^n$] is given as

$$R_1 \propto \exp \left\{ -\left(\frac{q}{kT}\right) \left[\left(\frac{1}{2}\phi_R + \frac{1}{4}\phi_D\right) - \frac{1}{2}aE_{ox} \right] \right\} \quad (3.17)$$

where ϕ_R is the enthalpy of the reaction (2.6), ϕ_D is activation energy of diffusion and E_{ox} is oxide field. As a result, the extracted Arrhenius activation energy should correspond to the interaction of these different reactions. Furthermore, it has been shown from Fig. 3.7 that oxide field accelerator has a negligible dependency on nitrogen. Therefore, another possible interpretation for the decreased E_a with nitrogen concentration is the weakening of Si-H bond by the nitrogen incorporation at the Si/SiO_xN_y. We hypothesize that the weakening effect could be linked to either due to its modification of Si-H neighboring bonding structure or increasingly interfacial strain due to excessive of nitrogen incorporation. This is not surprising since it has been proposed that interfacial strain plays an important role in Si-H bond dissociation [56], [112]. Furthermore, recent molecular orbital calculations have shown that nitrogen incorporation will increase the interfacial strain at the interface [113]. This is also consistent with the finding that the ΔV_{th} is dominated by the interfacial nitrogen and the role of nitrogen at the bulk oxide is insignificant. We will present more studies in the following chapters to understand the physical meaning of this E_a value.

3.6 Chapter summary

In summary, the influence of interfacial nitrogen concentration on the time, oxide field and temperature dependence of the NBTI-induced threshold voltage shift has been studied. It has been observed that nitrogen has negligible effect on time exponent and oxide field accelerator. However, nitrogen has a strong impact on the temperature dependence. Furthermore, both positive oxide charge and interface trap are confirmed to be the primary defects responsible for threshold voltage shift and device parameter degradation in both pure SiO₂ and nitrided oxides. Another important observation is that both positive oxide charge trapping and interface trap generation increase proportionally with interfacial nitrogen concentration and their ratio is approximately equal to 1. It is further observed that the charge trapping and the interface state generation have the same activation energy within the experimental errors for a given interfacial nitrogen concentration. In addition, their activation energies have been found to follow the same dependence on the nitrogen concentration, where the activation energies decrease linearly with interfacial nitrogen concentration. These results suggest that the charge trapping and the interface state generation have the same origin. In addition, by employing plasma nitridation, NBTI induced degradation can be minimized as compared to conventionally thermal nitridation technique. The suppression of NBTI is achieved by displacing the nitrogen peak profile away from the Si/SiO_xN_y interface hence improving the interfacial properties and reducing nitrogen content at the interface. A model on the electrochemical reactions, which lead to the oxide charge trapping and interface trap generation, is described, and some discussions on the nitrogen-worsen NBTI effect are presented

CHAPTER FOUR

Atomic Modeling of NBTI in SiO_2 and SiO_xN_y gate dielectrics using first-principles calculation

In this chapter, we present an atomic modeling of NBTI in SiO_2 and SiO_xN_y gate dielectrics using first-principles calculations. With the aid of experimental findings established in Chapter Three and from other reported literatures, we develop the NBTI atomic model. In this model, the possible origin of NBTI in both SiO_2 and nitrided oxides are discussed. In addition, the effect of nitrogen as a i) reaction site and ii) neighboring atom in NBTI are discussed. Consequently, the role of nitrogen in NBTI can be understood in terms of its electronegativity, atomic charge distribution and increasing initial interfacial defect density. Finally, NBTI is mainly a hydrogen-originated hole trapping reaction.

4.1 Introduction

It has been known that NBTI-induced threshold voltage shift increases with nitrogen content at the Si/SiO₂ interface. Although it is known that holes and hydrogen are involved in the degradation process, the mechanism on the atomic scale has not yet been clarified. Besides, the role of nitrogen on device degradation is not yet fully understood and it is still under debate. In addition, there is still lack of studies on the origin of NBTI in nitrided oxide; though it is generally accepted that interfacial defect like Si-H bond is one of them. For instance, Liu *et al.* [70] suggested that there is two different kinds of defect origins involved in NBTI degradation based on the observation that two different thermal activation energies result from two different stages of NBTI stress. In a more recent study, Mitani *et al.* [114] proposed that in addition to commonly accepted hydrogen-originated reactions, there are also hydrogen-unrelated structures such as twofold coordinated nitrogen, involve in the degradation process. Therefore, to suppress NBTI, one should understand the degradation reactions and origin of NBTI.

4.2 Origin of NBTI in pure and nitrided oxides

4.2.1 Role of Si-H in nitrided oxide

It has been commonly agreed that water, hydrogen and hole are involved in NBTI degradation for pure SiO_2 . Since thermal oxide is used for all the samples therefore, the role of water in nitrogen-worsen NBTI should be disregarded. To examine the role of Si-H in nitrided oxide, we prepare three nitrided samples with different post-metalization anneal (PMA) (i.e., forming gas anneal) conditions as depicted in Fig. 4.1. It can be seen that ΔV_{th} increases with longer duration of PMA. This is attributed to more hydrogen being incorporated in the $\text{Si}/\text{SiO}_x\text{N}_y$ interface. More importantly, skipping PMA results comparable NBTI performance between nitrided oxide and pure SiO_2 . A comparison of NBTI-induced interface trap and positive oxide charge density between nitrided oxides with and without PMA is shown in Table 4.1. It can be clearly seen that both ΔD_{it} and ΔN_{ox} are higher for oxide with PMA than oxide without PMA. Therefore, it can be concluded that nitrogen loses its enhancement effect without the aid of PMA and both nitrogen and hydrogen must co-exist for the enhancement effect. In another word, nitrogen-worsen NBTI is still a hydrogen-originated process.

Since, both nitrogen and hydrogen must co-exist in order to have the NBTI enhancement effect, it would be interesting to find out whether nitridation will increase the interfacial defects such as Si-H. This is imperative as Si-H is commonly accepted as precursor of NBTI. To do this, a short loop experiment is carried out to study the as-grown nitridation-induced interfacial defects. The split table is shown in Table 4.2. After post nitridation annealing, the as-grown interface trap density is analyzed with a non-contact surface photo-voltage technique [115]-[117].

Figure 4.1: The effects of post-metalization anneal on NBTI for nitrided oxides. For comparison, pure SiO₂ is included.

Table 4.1: Comparison of NBTI-induced interface trap and positive oxide charge density for nitrided oxide with and without PMA.

	$\Delta D_{it} (x10^{10} \text{ cm}^{-2} \text{ eV}^{-1})$	$\Delta N_{ox} (x10^{10} \text{ cm}^{-2})$
With PMA	7.66	10.67
W/o PMA	5.59	8.05

The as-grown interface trap density D_{it} as a function of N_{int} is shown in Fig. 4.2. One can clearly see that the as-grown D_{it} values before PMA are in the order of $10^{11} \text{ cm}^{-2} \text{ eV}^{-1}$. Being in good agreement with as-grown D_{it} values reported in [118]. In addition, it can be found that the as-grown D_{it} increases monotonically with interfacial nitrogen concentration. This can be explained by the well-established constraint bonding theory

[119]-[122]. Indeed, Lucovsky et al. [122] have shown that the density of defects at the Si/SiO_xN_y interface increases with the N_{int} , since bonding constraints at this interface are more important when N_{int} increases. The observed increase of as-grown D_{it} with N_{int} is thus consistent with the increase in bonding constraints induced by the presence of nitrogen. Besides, as can be seen from Fig. 4.2, post nitridation anneal (PNA) in N₂/O₂ ambient can anneal out the as-grown D_{it} partially.

Table 4.2: Split table for study of as-grown nitridation-induced interfacial defects.

	Rapid Thermal Oxidation	NO Nitridation (Interfacial nitrogen concentration)	Post Nitridation Anneal (PNA)
Sample 1	1.8 nm	4.5 at. %	skip
Sample 2	1.8 nm	4.5 at. %	1050C N ₂ /O ₂
Sample 3	1.8 nm	5.5 at. %	1050C N ₂ /O ₂
Sample 4	1.8 nm	7.5 at. %	1050C N ₂ /O ₂
Sample 5	1.8 nm	8.5 at. %	1050C N ₂ /O ₂

Figure 4.2: As-grown D_{it} as a function of interfacial nitrogen concentration.

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The interfacial Si-H bonds can then be produced from the fabrication sequence in which the as-grown D_{it} are created during nitridation process, and later passivation during post-metallization annealing in forming gas. They then act as precursors for NBTI stress as shown in Table 4.1. These results provide experimental evidence for the NBTI model [123], [124] prediction that nitrogen increases initial interfacial Si-H density. In addition, it can be concluded that not only nitridation and post-metallization anneal have a strong impact on NBTI, but also an optimized post nitridation anneal is also equally important in suppressing NBTI.

4.2.2 Role of vacancy defect in pure and nitrided oxide

On the other hand, neutral vacancy defect (V_o) can be generated at the interface and in the oxide due to growth, deposition, and doping processes and it has long been known to be the dominant intrinsic defect in amorphous SiO_2 [125], [126]. During stress, they can capture holes and become positively charged, contributing to ΔV_{th} just like NBTI-induced defects. Therefore, it is attractive to find out whether such a defect plays a role in NBTI degradation. For this purpose, five different atomic models are created as the precursor clusters for vacancy formation and are shown in Fig. 4.3. In the figure, structures (i) and (ii) are used as references, and structures (iii) to (v) are employed to illustrate the impact of N as first-nearest-neighbor (1^{st} -NN) on vacancy formation since the number of N atoms surrounding Si increases with higher nitrogen content [127], [128].

First-principles calculations were then performed for the five atomic models in the framework of a linear combination of hybrid gradient-corrected density functional theory with Becke's exchange function [85] and the Lee–Yang–Parr correction function [86] for

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all electronic structure calculations. The electronics structure is expanded using a mixed Gaussian basis set with split-valence-type plus polarization basis set [6-31g(d)] on all atoms. In the geometry optimization process, optimization converges to a structure on the potential energy surface where forces on the system are essentially zero. However, the final structure may correspond to a true minima or a saddle point. Therefore, after the geometry optimization calculation, a frequency analysis was performed to confirm the true minima and first-order saddle points. After atomic relaxation for reactants, we obtained Si-N bonds of 1.75 ± 0.02 Å and Si-O bonds of 1.65 ± 0.01 Å, being consistent with previous calculations [129], [130]. This suggests that our relaxed models give a good representation of the local structure for various bonding configurations.

In each case, the vacancy defect in oxide film is generated by removing the bridging oxygen atom from its site in the various relaxed perfect molecule clusters shown in Fig. 4.3, followed by full relaxation of all remaining atoms. The main effect of the relaxation is the formation of a Si-Si dimer bond with a length ranging from 2.332 Å to 2.360 Å for all the structures studied here. These bond lengths are substantially shorter by about 0.711 to 0.750 Å than those between two Si atoms prior to the vacancy defect formation. This is consistent with the common feature for vacancy defect formation that the two Si atoms adjoining the vacancy move inward [131]-[133]. The rest of the network experiences marginal changes upon relaxation. This suggests that adding N into the SiO₂ causes insignificant structure change upon vacancy defect formation.

Figure 4.3: Defect free oxide cluster models in SiO_2 and SiO_xN_y films. To form a vacancy defect, a bridging O atom (as shown in the arrow) is removed and the structures are allowed to relax. Vacancy formation energy $E_f(V_o)$ is also compared and given in the figure. The unit for energy is in eV.

The vacancy formation energy $E_f(V_o)$ is obtained from the calculation of the total energy difference between the perfect neutral structure, $E_t(\text{SiO}_2)$ and the sum of fully relaxed neutral vacancy cluster, $E_t(V_o)$, and an isolated oxygen atom, $E_t(O)$. This is shown as follow:

$$E_f(V_o) = [E_t(V_o) + E_t(O)] - [E_t(\text{SiO}_2)] \quad (4.1)$$

In this way, one can determine the formation energy for different molecule clusters and the results are shown in Fig. 4.3. From Fig. 4.3, the formation energy for structure (ii) is

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higher than structure (i) by 0.77 eV. This indicates that, although neutral oxygen vacancies are energetically unfavorable in both structures, their creation is easier at the Si/SiO₂ interface than in the bulk oxide. This implies that, if an oxygen deficient situation happens during the oxide growth, oxygen atoms will migrate from the interface. In this way, vacancies are created at the Si/SiO₂ interface towards the bulk oxide, healing the oxygen vacancies in the bulk oxide. Furthermore, increasing the number of N as 1st-NN to the vacancy results in marginal changes in the vacancy formation energy, indicating that incorporation of N does not substantially increase the concentration of the V_o defects.

To understand whether vacancy defects are responsible for the nitrogen-worsen NBTI-induced ΔV_{th} , Fig. 4.1 provides such an answer. This is because hydrogen post-metallization annealing (PMA) in forming gas can terminate the vacancy by forming H-complexed O vacancy ($\equiv\text{Si-H H-Si}\equiv$). Based on Fig. 4.1, it can be observed that ΔV_{th} without PMA is lower than that with PMA but is comparable to that of pure SiO₂. This indicates that NBTI degradation is reduced due to the absent of Si-H bond. Therefore, the result suggests that the hole trapping in V_o, which should appear more in the sample without PMA, does not play a crucial role in nitrogen-worsen NBTI. This is also partly attributed to the fact that the concentration of vacancy defects is lower than the concentration of hydrogen related defects (e.g. Si-H) in an optimized fabrication process.

4.3 Atomic model of NBTI in pure and nitrided oxides

4.3.1 Discussion on prevailing NBTI models on nitrogen effect

As reviewed in Chapter Two, the model of NBTI electrochemical reactions in pure SiO_2 predicts that the interface trap and positive oxide charges are generated from the dissociation of hydrogen terminated trivalent Si bonds (Si-H) by holes in the Si inversion layer during NBTI stress. The balance between these competing processes determines the net generation of defects. When the concentrations of the released hydrogen species decrease, the reactions tend to favor the generation of interface states and/or the fixed charges accordingly. Although this model is derived to explain the $t^{0.25}$ that is commonly observed in time dependence of NBTI degradation, however, these electrochemical reactions are inadequate to explain the nitrogen-worsen NBTI effect because they do not take into account the effect of nitrogen at the Si/ SiO_xN_y interface. In a recent theoretical study, Ushio *et al.* [134] considered the effect of nitrogen at the interfacial layer and proposed that nitrogen-worsen NBTI effect is related to the higher stability of hole trapping states at the Si/ SiO_xN_y interface than that at the Si/ SiO_2 interface. However, their mechanism is not consistent with the finding that the net defect generation rate is determined by the concentration of released hydrogen species. Furthermore, as demonstrated in Fig. 4.1, both nitrogen and hydrogen must co-exist to produce the enhancement effect in ΔV_{th} . On the other hand, Houssa *et al.* [123], [124] considered that the nitrogen would increase the concentration of interfacial defects since average coordination number increases with nitrogen based on the well-established constraint theory [119]-[122]. As a matter of fact, our experimental results from Fig. 4.2 agree excellently with this prediction. In addition, they proposed that nitrogen would increase the distribution of Si-H dissociation energy due to enhancement of interfacial

strain by nitrogen. However, they only consider the effect of nitrogen on interface trap generation and neglect the positive oxide charge generation during NBTI though its contribution to threshold voltage shift is significant. Furthermore, they have not yet provided experimental or theoretical calculation to support their model.

4.3.2 Atomic modeling of nitrogen-worsen NBTI

To consolidate the various results by others and us, we propose that the nitrogen-worsen NBTI effect is related to both hydrogen-originated and diffusion-controlled electrochemical reactions. In this model, Si-H bond is the origin of NBTI in pure SiO₂ as well as in nitrided oxide based on the finding obtained from Fig. 4.1. On the other hand, it has been observed that the time exponent factor t^n ($n \sim 0.20$) has negligible dependence on nitrogen (Fig. 3.5), and therefore the factor is attributed to diffusion-controlled electrochemical reactions [31], [35], [50]. In this scenario, the electrochemical reactions for both pure and nitride oxide are of the following forms:

Since NBTI-induced N_{ox} and N_{it} generation have a linear correlation regardless of the nitrogen concentration as shown in Figs. 3.9, 3.12 and 3.13. Then overall NBTI electrochemical reaction can be re-formulate in the following forms of **hydrogen-originated hole trapping reactions (or NBTI reactions)**:

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Firstly, the interface traps (Si•) are generated from the dissociation of hydrogen terminated trivalent Si bonds (Si-H) by interaction with holes (h^+) in the Si inversion layer during NBTI stress. It is worth mentioning that this mechanism is consistent with theoretical models that predict lower activation energies for hydrogen dissociation from Si-H when charged states exist [56]. Then the released hydrogenated species (H^+) diffuse and are trapped near the oxide interface resulting in the positive oxide charges (Si-OH⁺-Si or Si-NH⁺-Si). This is also supported by a recent experimental result which demonstrates that released hydrogen species is redistributed and accumulated at or near the oxide substrate interface during NBTI stress [135]. In addition, using the plasma nitridation, we have established that nitrogen at the interface plays a significant role in NBTI whereas nitrogen at bulk oxide plays a trivial role (Figs. 3.18 and 3.19). Note that in both cases (i.e. reactions 4.6 and 4.7), the hydrogen-related structures act as the common origin for both interface trap and positive oxide charge generation, being consistent with the observation that oxide charge and interface trap generation have the same activation energy as depicted in Fig. 3.16.

Therefore, based on the proposed atomic model, we ascribe the nitrogen-worsen NBTI effect to the enhancement of the trapping of the hydrogen ions (H^+), which are released from the reaction (4.2), near the interface by the incorporation of nitrogen. In other words, reaction (4.5) is easier to occur than reaction (4.4). The enhancement of the trapping effect would favorably shift the equilibrium state to the right-hand-side of reaction (4.7), leading to a faster generation of interface trap and oxide charge. It should

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be pointed out that this model is consistent with prevailing models in pure SiO_2 as the net defect generation still depends on the concentration of released hydrogen species.

To support our hypothesis, we have performed first-principles calculations to show the effects of nitrogen on the trapping of hydrogen species at the interface. The methodology is similar to that in section 4.3.2. We have also confirmed that our relaxed models give a good representation of the local structure for various bonding configurations by comparing our bond length with those reported in literature [129],[130].

Figure 4.4: Cluster model of the Si/SiO_2 and $\text{Si}/\text{SiO}_x\text{N}_y$ interface structures. The reaction energies (E_R) for the trapping of the hydrogen ions (H^+) are obtained from first-principles calculations after performing geometry optimization on both reactants and products. The numbers in the figure is the bond length (in angstrom) for the respective bonds.

The reaction energy E_R for the hydrogen ion trapping/migration at interfaces is calculated with the cluster models shown in Fig. 4.4. For the $\text{Si}/\text{SiO}_x\text{N}_y$ interface structure, the nitrogen atom is in the Si_3N configuration [129]. Geometry optimization

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for both reactants and products has been performed prior to E_R calculation. E_R is calculated by subtracting the total molecular energy before reaction from that after the reaction, and the result is also indicated in Fig. 4.4. The E_R is -8.51 and -9.54 eV for Si/SiO₂ and Si/SiO_xN_y interface structures, respectively. It can be seen that H⁺ trapping process is exothermic, and more negative E_R implies that the reaction occurs more readily. Hence, the likelihood of H⁺ being trapped at Si/SiO_xN_y interface is higher than that at Si/SiO₂ interface. In this scenario, H⁺ is trapped at the interface to form a more stable state by accommodating a lone electron pair either from the O center for pure oxide or N center for nitrated oxide. H⁺-trapping leads to more dissociated H ions generation due to the shift of equilibrium state of reaction (4.6). N is less electronegative than O and would thus be more inclined to share the lone pair. Therefore, N lone pair is a better donor than O lone pair. In other word, N atom is an effective hydrogen trapping center as compared to O atom. Furthermore, upon trapping of H⁺, the over-coordinated complexes weaken the interface by the elongation of Si-O and Si-N bond lengths as indicated in Fig. 4.4. This weakening interface will continue to pose serious reliability problem to pMOSFETs.

It is worth mentioning that the discussion on nitrogen-worsen NBTI effect can be accomplished without knowing whether the diffusion species are H⁰ or H⁺. As the difference of the reaction energies for the trapping between hydrogen atoms and hydrogen ions corresponds to the ionization energy of a hydrogen atom. Therefore, it is obvious that the reaction energy of the trapping of hydrogen atom (H⁰) at Si/SiO_xN_y interface is also lower than that at Si/SiO₂ interface. Therefore, it can be concluded that the trapping of both H⁺ and H⁰ is enhanced by the nitrogen incorporation at the interface, and this leads to the enhancement of both the interface trap and positive oxide charge generation as discussed above.

4.3.3 Atomic modeling of nitrogen neighboring effect on NBTI

Although we propose that trapping of dissociated hydrogen species from Si-H might be responsible for the nitrogen enhancement effect. The trapping occurs more readily at N sites than at O sites, giving rise to more defect generation at Si/SiO_xN_y interface. However, these studies have not covered all possible N bonding configurations (note that the number of N atoms surround a Si atom is a function of nitrogen concentration). Such a study in this aspect is important, as gate oxide with higher nitrogen content will be used in future generation CMOS devices.

Furthermore, results from Figs. 3.11(b) and 3.12(b) show that both NBTI-induced N_{ox} and N_{it} generation increase linearly with the interfacial nitrogen concentration up to $N_{int} \sim 8$ at. %. As more nitrogen is required as technology moves into advanced regime, the relationship between the N_{int} and the NBTI-induced ΔV_{th} beyond 8 at. % would be of great interest. For this purpose, we prepared additional three nitrided oxides with interfacial nitrogen concentrations of 8.5, 12.5 and 15.5 at. % in addition to the seven samples used in Chapter Three. Figure 4.5 depicts the experimental ΔV_{th} and prefactor A caused by a 1000 s NBTI stress as a function of the nitrogen concentration up to 16 at. %. It is observed that both ΔV_{th} and prefactor A follow the same dependence on N_{int} indicating a link between them. On the contrary, the time exponent factor n has a weak dependence on the N_{int} and is about 0.2 in average. The weak dependence of the exponent factor n suggests that the degradation mechanism of highly nitrided oxides is still related to diffusion-controlled electrochemical reactions. More importantly, as shown in Fig. 4.2, the N_{int} dependence has two linear regions with different slopes (i.e. the region for $N_{int} < 8$ at. % and another region for $N_{int} > 8$ at. %). Obviously, the dependence for the region of $N_{int} > 8$ at. % is stronger than that for the region of $N_{int} < 8$ at. %. As discussed later, this

N_{int} dependence can be explained in terms of the N neighboring effect with the scenario that the one-N atom structure (N-Si-O_3) is dominant for $N_{\text{int}} < 8$ at. % but the two-N atoms structure ($\text{N}_2\text{-Si-O}_2$) becomes dominant for $N_{\text{int}} > 8$ at. %.

Figure 4.5: Dependence of ΔV_{th} and prefactor A on N_{int} . The NBTI stress was $V_g = -2.2\text{V}$ at temperature of 125°C .

It has been clear from the first-principles calculations that reaction (4.7) is easier to occur than reaction (4.6) due to the enhancement of H^+ trapping near the interface by nitrogen. It is also clear from Fig 4.5 that the NBTI degradation increases with the N_{int} . On the other hand, it has been reported that the number of N atoms surrounding a Si atom increases with N_{int} [127], [128]. More notably, it is found that a bond structure in which one of the four surrounding O atoms is replaced by a N atom (i.e., N-Si-O_3) is dominant when N_{int} is less than 8 at. % [127]. However, when N_{int} is increased beyond 8 at. %, a structure where two N atoms are bonded to one Si atom (i.e., $\text{N}_2\text{-Si-O}_2$) emerges and

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becomes dominant when N_{int} goes beyond 10 at. % [127]. This analysis coincides excellently with the observation in Fig. 4.5. This strongly suggests the important role of N neighboring effect in the nitrogen-worsen NBTI.

To understand the role of the neighboring effect, first-principles calculations are carried out to determine the reaction energies of the above reactions (4.7) with one of the chemical structures (N-Si-O₃, N₂-Si-O₂, N₃-Si-O, and N₄-Si) involved. For comparison, the result NBTI in pure SiO₂ is included (i.e. reaction 4.6). In this case, one of the four surrounding O atoms is gradually replaced by N atom for the study of neighboring effect. The corresponding molecular clusters and reactions are shown in Fig. 4.6. After performing geometry optimization of both reactants and products, reaction energy of each reaction is obtained by subtracting the total molecular energy before reaction from that after the reaction and is given as

$$E_R = (E_{t,N_{ox}} + E_{t,N_{it}}) - (E_{t, Si-O-Si} + E_{t, Si-H}) \quad (4.8)$$

where E_t is the total molecular energy for respective clusters and obtained from first-principles calculations. We compare the E_R for these reactions and their relative reaction energies ΔE_R are shown in Fig. 4.6. The negative ΔE_R indicates that the NBTI reaction in nitrided oxides is more favorable than that in pure SiO₂. It is found that the ΔE_R decreases with increasing the number of N atoms surrounding a Si atom, indicating that the reaction is easier with more neighboring N atoms.

An actual Si/SiO_xN_y interface may contain the chemical structures of O₄-Si, one-N and two-N atomic structures [i.e., N-Si-O₃ and N₂-Si-O₂], assuming that the contributions of the three-N and four-N atomic structure are negligible [127]. Therefore, the NBTI reaction energy for such an actual Si/SiO_xN_y interface can be expressed as:

$$E_R = (1-N_1-N_2) E_{R,0} + N_1 E_{R,1} + N_2 E_{R,2} \quad (4.9)$$

Figure 4.6: Relative reaction energies (ΔE_R) of NBTI reaction at Si/SiO₂ interface and Si/SiO_xN_y interface [reactions (i)-(iv)].

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where $E_{R,0}$, $E_{R,1}$ and $E_{R,2}$ are the reaction energies for the reactions involving the chemical structures of $\text{O}_4\text{-Si}$, one-N atomic structure and two-N atomic structure, respectively, and their values are obtained from Fig. 4.6. Here, N_1 and N_2 denote the atomic percentages of the one-N and two-N atomic structures, respectively, in the nitrated oxide. Therefore, for a given N_1 and N_2 , the reaction energy for a nitrated oxide can be calculated with Eq. (4.9). Fig. 4.7 shows the relative reaction energy (ΔE_R) as a function of N_1 or N_2 .

Figure 4.7: Dependence of relative NBTI reaction energy on N_1 and N_2 .

As can be seen in Fig. 4.7, the ΔE_R decreases as N_1 or N_2 increases, which strongly suggests the enhancement of the NBTI degradation by nitrogen. On the other hand, Fig. 4.7 shows that the reduction of the E_R with N_2 is faster than that with N_1 . The E_R reduction rate for N-Si-O₃ is $\left| \frac{\partial(\Delta E_R)}{\partial N_1} \right| = 10.3 \text{ meV / at.\%}$ while it is $\left| \frac{\partial(\Delta E_R)}{\partial N_2} \right| = 11.9 \text{ meV / at.\%}$ for N₂-Si-O₂. This clearly spells the N-neighboring effect, i.e., the reduction of reaction energy with increasing interfacial nitrogen concentration is faster when the N₂-Si-O₂ is

dominant than that when N-Si-O₃ is dominant. This means that the enhancement of the NBTI degradation by nitrogen is more significant when two-N atomic structure, N₂-Si-O₂, is dominant ($N_{int} > 8$ at. %) than that when one-N atomic structure, N-Si-O₃, is dominant ($N_{int} < 8$ at. %). Obviously, such a mechanism satisfactorily explains the N_{int} dependence of the ΔV_{th} and prefactor A shown in Fig. 4.5.

4.4 Atomic model of NBTI in pure and nitrated oxides with defects

It has been demonstrated in section 4.2.2 that vacancy defect plays a trivial role in nitrogen-worsen NBTI for a properly optimized gate dielectrics. This is partly because the concentration of the vacancy defect is lesser than that of hydrogen-related defects (i.e. Si-H). However, it is still interesting to find out whether NBTI is energetically favorable in such a defective oxide as compared to the situation in defect-free oxides. Furthermore, the defect has also been widely accepted as the hole trapping center, therefore, the effect of nitrogen on hole trapping reaction would be of interest.

4.4.1 Effect of nitrogen on hole trapping at vacancy defect

To study the effect of N on hole trapping by oxygen vacancy, several positively charged oxygen vacancies (V_o^{+1}) are created by removing an electron from the V_o centers described in section 4.2.2 [i.e. structures (ii) to (v) in Fig. 4.3]. After the creation of the positive charge, each model cluster is allowed to relax to give a minimum energy configuration. Similarly, a frequency analysis is carried out to confirm the true minimum state. After relaxation, the two Si atoms forming a dimer bond move slightly away from

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each other, by 0.263 Å (16 % of Si-O distance) for structure (ii) and linearly down to 0.146 Å for structure (v) (the structures are shown in Fig. 4.3). This indicates that neighboring N atoms reduce the structure disruption caused by hole trapping. Then the formation energy for hole trapping state, $E_f(V_o^{+1})$ is determined as follow:

$$E_f(V_o^{+1}) = E_T(V_o^{+1}) - E_T(V_o) \quad (4.10)$$

The $E_f(V_o^{+1})$ values for these structures are compared and shown in Fig. 4. 8. It can be seen that $E_f(V_o^{+1})$ is generally lower in SiO_xN_y than in SiO_2 . This means that increasing the number of N as first-nearest neighbor the vacancy leads to an easier hole trapping in the vacancies. Therefore, the Si/ SiO_xN_y interface with a larger N concentration could be more susceptible to the hole trapping. These results can be employed to explain the commonly observed nitridation-induced positive oxide charge.

Figure 4.8: Comparison of formation energy for hole trapping reaction at vacancy defects in SiO_2 and SiO_xN_y films. Note that Si---Si is the vacancy defect.

4.4.2 Effect of nitrogen on hydrogen-originated hole trapping reaction (NBTI) at vacancy defect

Since the N atoms adjacent to the V_o can lead to an energetically favorable hole trapping state, let's focus on the study of hydrogen-originated hole trapping reaction or NBTI (note that these terms are interchangeable) at the V_o . In this scenario, the V_o would acts as the trapping center and the overall electrochemical reaction is in the form:

To examine the energy of NBTI reaction in this vacancy defect and the role of nitrogen as first-nearest neighbor, we perform the calculation of NBTI reaction on defect structures (ii) to (v) describe in Fig. 4.3. Their reaction energies are shown in Fig. 4.9. For comparison, NBTI reaction energies for defect-free structures are included. The negative ΔE_R indicates that the NBTI reaction is more favorable than that in pure SiO₂. As shown in Fig. 4.9, both cases (i.e. vacancy defect and O as hydrogen trapping center) the ΔE_R decrease with increasing the number of N atoms surrounding a Si atom, indicating that the reaction is easier with more neighboring N atoms. This is consistent with the N neighboring effect shown in Fig. 4.6. To have a better view on the effect of nitrogen, the ΔE_R of NBTI reaction is plotted as a function of the number of N as 1st-nearest neighbor (1st-NN) for three different hydrogen trapping sites, namely, O, N and V_o , as shown in Fig. 4.10. At the first glance, nitrogen is detrimental to NBTI for all cases. It is interesting to note that although N is an effective hydrogen trapping center than O, they follow a similar dependence on nitrogen neighboring effect as one can see from their slope in Fig. 4.10. More notably, hydrogen trapping at vacancy has the strongest dependence on nitrogen neighboring effect.

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(a) NBTI at defective interface (vacancy defect as reaction site)		$\Delta E_{\text{R NBTI}}$
(i)	-0.02 eV
(ii)	-0.40 eV
(iii)	-0.67 eV
(iv)	-1.00 eV
(b) NBTI at defect-free interface (O as reaction site)
(v)	0.0 eV
(vi)	-0.27 eV
(vii)	-0.45 eV
(viii)	-0.61 eV

Figure 4.9: Effect of nitrogen on (a) NBTI reaction energy at defective interface i.e. vacancy defect acts as hydrogen trapping center; and (b) NBTI reaction energy at defect-free interface, i.e. O acts as hydrogen trapping center.

Figure 4.10: ΔE_R as a function of the number of N as 1st-nearest neighbor for three different hydrogen trapping centers, namely, vacancy defect, oxygen and nitrogen.

The strongest dependence on N neighboring makes the vacancy defect a more effective trapping center than oxygen trapping center. Nevertheless, this situation hardly occurs in practice as vacancy defect and hydrogen cannot co-exist and vacancy defect density is always reduced through annealing in an optimized fabrication process. Moreover, it has been demonstrated in section 4.2.2 that incorporation of nitrogen would not significantly increase the concentration of vacancy defect. Therefore, practically, vacancy defect plays an insignificant role in hydrogen-originated hole trapping reaction. Nevertheless, this result indicates that the nitrogen-worsen ΔV_{th} would be persisted in un-optimized fabrication process, probably through hole trapping reaction or hydrogen-originated hole trapping reaction as shown in Figs. 4.8 and 4.9.

4.5 Understand of nitrogen-worsen NBTI from atomic charge distribution

Interface cluster model for hydrogen trapping center		Mulliken atomic charge analysis	Natural Population Analysis	Electrostatic potential based on Chirlian-Francel model
O1	-0.6242e	-1.2505e	-0.869e
	Si2	+0.5958e	+1.2437e	+1.3157e
	Si3	+1.0831e	+2.4109e	+1.6779e
N1	-0.8138e	-1.747e	-1.0104e
	Si2	+0.5103e	+1.1296e	+1.1649e
	Si3	+0.4938e	+1.1302e	+0.9696e
	Si4	+1.0763e	+2.3986e	+1.5571e

Figure 4.11: Comparison of atomic charge for oxygen and nitrogen as hydrogen trapping center based on three different analysis methods, namely, Mulliken atomic charge analysis, Natural Population Analysis and Chirlian Francel model.

It has been demonstrated that N is less electronegative than O and would thus be more inclined to share the lone pair. Therefore, nitrogen lone pair is a better donor than oxygen lone pair and hence an effective hydrogen trapping center. On the other hand, to provide further insight into the effect of nitrogen neighboring effect, we calculate the

atomic charge from three different methods, namely, Mulliken Analysis [93], Natural Population Analysis [94] and Chirlian Francel model [96] for oxygen and nitrogen acting as trapping center as shown in Fig. 4.11. From a comparison among them, it is immediately clear that due to dipole effect, all three methods assign bridging O and N atom with negative charge whereas the Si atoms are positively charged. Hence, it is expected that these bridging atoms provide a Coulombic attraction center for trapping of positive charge like H^+ in this scenario. Moreover, computation from all three methods consistently shows that N has larger negative atomic charge than O. This means N is a more efficient trapping center for H^+ . Therefore, as number of N surrounding Si atoms increase, the localized structures would have a higher Coulombic attraction force for H^+ . This spells the nitrogen neighboring effect.

4.6 Understand of NBTI-induced defect structure

Up to now the BTI-induced defects have only been practically understood in the light of practical experiment, therefore the need for further study on defect structure in atomic scale is imperative. Such a study would be useful, as an understanding of defect structure would give insights into the evolution of device degradation during post-NBTI stress. From previous sections it have been clear that the formation of a positive charge state upon trapping of dissociated hydrogen species originates from the breaking of the Si-H bonds at the Si/ SiO_2 interface during NBTI stress. This positive charge state is responsible for the threshold voltage shift and device speed reduction. In addition, an elongation of localized bond lengths is observed as shown in section 4.3.2. This indicates that the bond strength is weakened upon the formation of NBTI-induced defect. Figure 4.12 illustrates the band gap modification of the molecule cluster before and after the

NBTI effect. Based on the first-principle calculations, the band gap of the cluster is reduced by 0.21 eV after NBTI (i.e. after trapping of a H^+ by the oxygen center). Here, the band gap is defined as the difference between eigenvalues of highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) for the frontier molecular orbital of the structures shown in Fig. 4.12.

Figure 4.12: Comparison of the SiO_2 interfacial band gap before and after H^+ trapping.

The structures of the interfacial species considered are shown.

The calculated energy diagrams in Fig. 4.13 show the schematic band structure of the reactants and products. Activation energy required for the reaction is denoted by E_A and is not drawn to scale. The energy levels of the HOMO and LUMO for the respective species in Figure 4.12 are as indicated, with the frontier molecular orbital energy gap located between the HOMO and LUMO. The remaining molecular orbitals are represented with blocks, where orbitals below the HOMO are filled states while that above the LUMO are empty states. The H^+ proton is perceived as an isolated atomic

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species hence the electronic structure is depicted as discrete energy levels with two energy levels, LUMO and LUMO_{-1} . In its elemental state, each hydrogen atom has one unpaired electron, which occupies a stable, low-energy orbital. After breaking of the Si-H bond by a hole, H^+ is formed by removing one electron from H, in the process vacating this low-energy orbital, which becomes the LUMO of H^+ . The original LUMO hence becomes the LUMO_{-1} . H^+ migrates to the Si/ SiO_2 interface and acquires a more stable state by accommodating a lone electron pair from the oxygen center in its empty LUMO orbital, in the process forming a coordination bond (i.e both electrons used to form the bond are contributed by O and none from H).

Figure 4.13: Illustration of relative energy levels of the HOMOs and LUMOs for the three species involved in H^+ trapping at the Si/ SiO_2 interface. Structures of the species corresponding to each band diagram are depicted above the band diagram. The reaction energy pathway for the overall reaction is incorporated into the band structure diagrams.

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In this scenario, the electron transfer will take place from the HOMO of the electron donor (i.e. Oxygen in SiO₂) to the LUMO of the electron acceptor (i.e. H⁺) because the HOMO is the unstable filled state while the LUMO is the most stable empty state. Since the calculated LUMO energy level offered by H⁺ is lower than that of the HOMO of SiO₂, stability is gained from occupying a more stable energy state. As a result, both the HOMO and LUMO of the product are stabilized after H⁺ trapping, as noted from the calculated decrease in energy of the HOMO and LUMO as illustrated in Fig. 4.13. In addition, it can be observed that the LUMO of the product falls within the band gap of the oxide. This generates an energy state inside the band gap of the oxide, which can enhance tunneling if charge transfer is allowed through the state.

The decrease in band gap can be understood with the Weaire-Thorpe model [136], which proposed that the band gap of a tetrahedrally bonded group four element is controlled by two interplaying factors, namely the promotion energy cost for sp³ hybridization, Δ , and the energy gained from subsequent bonding, β . If the energy gain derived from tetrahedral bonding outweighs the energy required to hybridize the 3s and three 3p orbitals in Si into 4 sp³ hybrids, a band gap will be formed. Mathematically, the Weaire-Thorpe model predicts that a band gap will be formed if

$$|\beta| > 2|\Delta| \quad (4.12)$$

As such, it is clear that the original SiO₂ interface has a larger band gap, indicating a favorable bonding condition that can compensate the hybridization promotion energy cost. In the H⁺ trapping step illustrated in Fig. 4.13, any change in band gap after H⁺ trapping can be attributed to energy cost/ gain associated with formation of the OH⁺ bonding. The presence of a reduced band gap after H⁺ trapping suggests that the gain in bonding energy can outweigh the hybridization promotion energy cost but compared to

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the original SiO₂ structure, some energy gain from bonding in the original SiO₂ is compensated. This compensation of energy gain is likely to be associated with the formation of the OH⁺ bond and its effects on neighboring atoms. The postulation can be verified with the bond length changes of the Si/SiO₂ interfacial species before and after H⁺ trapping as depicted in Fig. 4.4). For example, before H⁺ trapping, the Si-O bonds closest to the O-trap center are 1.66Å and 1.64Å. This bond length increases to 1.82Å and 1.79Å respectively after H⁺ trapping. Elongation of bonds indicates weaker bond strength and poorer overlap of molecular orbitals, which results in poor interaction and hence lowered band gap, in agreement with the Weaier-Thorpe model. Nevertheless, the overall reaction is still favorable because the net gains in stability of H⁺ in bond forming and the overall stability gained by the structure after H⁺ trapping outweighs the loss in bond strength of the neighboring Si-O bonds.

This study has improved our understanding of NBTI-induced defect structure in atomic scale. Such elongation of bond (as a result of bond elongation, band gap is lowered) as induced from NBTI defect structure has significant impact on the reliability of the device. Indeed, it is found that the hot carrier stress damage at $V_g=V_d$ increases as temperature increases, contrary to conventional hot carrier behavior [137]. The cause of damage is identified as being NBTI-related, which is greatly accelerated under hot carrier stress condition. To demonstrate the NBTI-worsen hot carrier (HCI) degradation, Figure 4.14 shows a comparison of experimental HCI and NBTI-worsen HC (NBTI + HCI) degradation of *p*-MOSFET. For NBTI-worsen HC degradation, we employ an AC test pattern as shown in the inset of the figure. For comparison, a static HC stress is included. Note that the stress condition for the static HC is purposely chosen to be the subset of the AC test pattern shown in the inset of the figure. It is evident that threshold voltage shift

(ΔV_{th}) is one order larger in NBTI + HCI stressing mode. Hence, consistent with [137], HC degradation is indeed worsen by NBTI. It has been known that HC degradation depends largely on the localized electric field at drain edge and interfacial bond structures at SiO_2/Si . Therefore, we propose that NBTI-worsen HC degradation is due to 1) increase of localized electric field at drain edge as a result of NBTI-generated positive oxide charge and 2) bond weakening at the NBTI-induced defect structure as mentioned earlier on. Such a bond weakening due to NBTI-induced defects satisfactory explain this NBTI-worsen HC degradation. More results and discussion will be presented to illustrate the interaction between NBTI and HC degradation in Chapter 6.

Figure 4.14: Comparison of HCI degradation by static HCI and NBTI-worsen HCI. The static HCI is stressed at $V_{gs}/V_{ds} = -0.5/-2.2 \text{ V/V}$.

4.7 Chapter summary

In summary, an intensive atomic modeling of NBTI is presented. It is found that hydrogen-related defect e.g. Si-H is the origin for NBTI in pure SiO_2 and nitrided oxide. More importantly, nitrogen and hydrogen must be present for the enhancement of threshold voltage shift whereas vacancy defect plays a trivial role in NBTI. In addition, NBTI for both pure SiO_2 and nitrided oxide can be modeled by hydrogen-originated reaction. It has been demonstrated from first-principles total-energy calculation that nitrogen can be an efficient trapping center for hydrogen ion as compared to oxygen. Furthermore, the NBTI degradation dependence of N_{int} at two distinct regions, namely, $N_{\text{int}} > 8$ atomic % and $N_{\text{int}} < 8$ atomic %, can be explained in terms of the effect of N atoms surrounding a Si atom. With this N neighboring effect, the reduction of reaction energy for the NBTI reaction with increasing the N_{int} is faster when the two-N atoms structure ($\text{N}_2\text{-Si-O}_2$) is dominant than that when the one-N atom structure (N-Si-O_3) is dominant. This N neighboring effect on the enhancement of the NBTI degradation is detrimental to future generations of MOS devices that require higher N_{int} for the gate oxide. Based on the first-principles calculations, it is shown that neighboring N enhances both hole trapping and hydrogen-originated hole trapping reaction in vacancy defect.

Finally, one can conclude that effect of nitrogen in NBTI is two fold, i.e., it provides more reaction sites (N trapping centers) or precursors (Si-H bond as shown in section 4.2.1), and it enhances the NBTI reaction by reducing the reaction energy as compared to oxygen. This can be understood from the fact the nitrogen is less electronegativity than oxygen and a larger negative charge at nitrogen atom provides a more effective Coulombic attraction center for trapping of positive charge like H^+ . Therefore, this study justifies the hypothesis in Chapter Three that incorporation of

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nitrogen enhances the trapping of the dissociated hydrogen species at the $\text{Si}/\text{SiO}_x\text{N}_y$ interface. Additionally, the impact of NBTI-induced defect structure is studied. It is found that after NBTI, the localized structure is weakened, gap state is generated within the oxide band gap and the oxide band gap is lowered. This poses a serious threat to another reliability issue like hot carrier issue.

CHAPTER FIVE

Impact of strain and oxide stoichiometry on NBTI

This chapter presents an experimental and theoretical study to on the impact of interfacial strain and oxide stoichiometry on NBTI. By comparing the NBTI degradation of steam oxide and dry oxide, the influence of interfacial strain on NBTI degradation emerges. In addition, the width dependence of NBTI reveals another aspect of mechanical stress-enhanced NBTI degradation. Furthermore, from the study of gate dielectric thickness-dependence of NBTI thermal activation energy, the importance of relaxing interfacial strain is emphasized to avoid reduction of NBTI activation energy. The experimental results corroborate the First-Principles study on the impact of interfacial strain and oxide stoichiometry on NBTI. From theoretical calculation, the Si-H bond strength is found to be sensitive to both interfacial strain and oxide stoichiometry but the former has a higher impact on the bond strength. Nevertheless, the bond is weaker in sub-stoichiometric oxide but stronger in stoichiometric oxide, and it is slightly weaker at the Si/SiO_xN_y interface than at the Si/SiO₂ interface. On the other hand, interfacial strain can deteriorate the hydrogen-originated hole trapping reaction while oxide stoichiometry has insignificant influence on the reaction. In short, the relaxation of the strained-layer is a more requisite issue in improving reliability and in realizing aggressive scaling.

5.1 Introduction

For decades, thermally grown, amorphous SiO_2 has been used as the dielectric material in metal-oxide-semiconductor (MOS) transistor [138]. Its extensive use is justified by the high quality, and the thermodynamically and electrically stable interface formed between thermally grown SiO_2 and the Si substrate [139]. With aggressive scaling of MOS devices, the dielectric/substrate interface becomes critical. According to Moore's scaling law, the gate oxide thickness in future generations of MOS devices will be less than 2 nm indicating that the dielectric/semiconductor interface will constitute a significant part of the device. Since the nature of the oxide/semiconductor interface differs significantly from the bulk properties of the oxide, understanding the SiO_2/Si interface structure and its dependence on the process conditions has become a topic of paramount importance [139], [140]. Therefore, considering the presence of a transition layer at the interface, an ultra-thin oxide layer can no longer be considered as homogeneous [141], [142].

The two major issues associated with thermally grown ultra-thin silicon dioxide films are the presence of sub-stoichiometric oxides (suboxides) [143], [144], and stress/strain near the oxide/substrate interface [140], [145]. Stress/strain near the Si/SiO_2 interface results from a lattice mismatch between the substrate and the oxide (intrinsic stress) and the difference in the thermal expansion coefficients of the two materials (thermal stress) [140]. Pasquarello *et al.* have quantified the strains based on a Si/SiO_2 interface model calculations and concluded that the strain is largely localized within the transition region [145]. The compressive stress degrades device performance by increasing the defect states near the interface [146]. Sub-stoichiometry at the oxide/substrate interface is present in the form of intermediate oxidation states of Si (Si^{1+} ,

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Si^{2+} and Si^{3+}), and the presence of suboxides may also have a similar undesirable effect [138]. Therefore, as the film thickness decreases, both strain and sub-stoichiometry might influence the reliability of transistor. However, majority of the studies in this context invoked only interfacial strain as the dominant factor responsible for the thickness dependent changes in the oxide breakdown [147]-[150]. Some also reported the impact of strain on hot-electron injection [152], [153]. Nevertheless, the impact of strain and sub-stoichiometry on NBTI has not been reported so far.

5.2 Experimental demonstration of the impact of interfacial strain and mechanical stress on NBTI

5.2.1 In-situ Steam Generated Oxide (ISSG) vs. Rapid Thermal Oxide (RTO)

It has been known that steam oxidation offers additional benefits as compared to dry oxidation. One of the most important features is that steam oxides have lower interfacial stress and fewer defects (pinholes, keyholes, micropores, etc.) than dry oxides. As a result, steam oxides have improved reliability, as measured by breakdown voltage and charge to breakdown [138], [147], [154]-[156]. In order to demonstrate the advantages offered by steam oxide over its thermally grown counterpart in terms of interfacial strain, we prepared two types of oxide using rapid thermal process (RTO) in O_2 and in-situ steam generation (ISSG) in H_2/O_2 ambient to investigate the impact of interfacial strain on NBTI. Both samples have the gate oxide thickness of 1.8 nm. Figure 5.1 compares the time dependence of NBTI-induced ΔV_{th} for the RTO and ISSG. The NBTI stress is carried out at $V_g = -2.2$ V, at a temperature of 125 °C. It is evident that ISSG can suppress NBTI-induced ΔV_{th} as compared to RTO. According to the model proposed in Chapter Four that higher hydrogen content would exacerbate NBTI, hence the result is unexpected as ISSG has more H content in the oxide film. Therefore, the only plausible explanation for this result is interfacial strain. It is known that steam oxide can have rapid relaxation of intrinsic stress due to the incorporation of Si-OH in the SiO_2 network and subsequently lowering of oxide viscosity [138], [154]. As a result, we hypothesize that a lower interfacial strain in the ISSG film is responsible for the reduced NBTI-induced ΔV_{th} , as compared to the RTO film.

Figure 5.1: Comparison of time dependence of NBTI-induced ΔV_{th} for dry and wet oxide grown by rapid thermal oxidation (RTO) and in-situ steam generation (ISSG), respectively.

5.2.2 Width dependence of NBTI

On the other hand, several studies have reported on width dependence of hot carrier reliability for MOS transistor with LOCOS isolation and attributed the worsening HC reliability to mechanical constraint arising from the proximity of the bird's beak structure [157], [158]. When the transistor is further scaled, there have been numerous reports showing that the fresh device characteristics and oxide breakdown can also be degraded by the presence of large mechanical stress [159]-[169]. The mechanical stress is originated from shallow trench isolation (STI) [159]-[165] and thin films [165]-[169].

To further understand the effect of mechanical stress on NBTI, we used pMOSFETs with different channel width to generate various level of STI-induced

mechanical stress and the result is presented in Fig. 5.2. As depicted in Fig. 5.2, the time dependence of NBTI-induced ΔV_{th} for three different channel widths is compared. It is apparent that NBTI-induced ΔV_{th} is enhanced in the narrow width pMOSFET. This result does not appear surprising, because it has been reported that hot carrier injection can be enhanced in the narrow width nMOSFET and the enhancement is attributed to increased mechanical stress arising from the STI [161]-[163],[165]. The stress is generated due to a difference in thermal expansion coefficient between Si and SiO₂ in the STI where a compressive stress develops and peaks at the active area/STI interface. Hence, as device width reduces, a higher stress will be experienced by the channel active area. Consequently, the analysis leads us to infer that the ΔV_{th} enhancement is a result of STI-induced stress in the narrow width transistor.

Figure 5.2: Time dependence of NBTI-induced ΔV_{th} for three different channel width MOSFETs. The channel length is 0.3 μm for all samples.

5.2.3 Gate dielectric thickness dependence of NBTI E_a

As mentioned earlier, when gate dielectric thickness scales down into the ultra-thin regime (< 4 nm), the transition layer near the SiO_2/Si interface plays an important role on oxide reliability. In particular, the TDDB activation energy has been experimentally observed to reduce with increasing interfacial strain (compressive stress) [147]. Figure 5.3(a) depicts the gate dielectric thickness T_{ox} dependence on NBTI thermal activation energy and interfacial strain. Note that the interfacial strain is the average strain value and is re-plotted using the data from [154]. From Fig. 5.3(a), it is observed that in general E_a decreases with T_{ox} . The E_a decrement is more rapid for T_{ox} less than 2 nm. Coincidentally, the average interfacial strain (compressive) is found to increase with decreasing T_{ox} and increment is more severe for T_{ox} less than 2 nm. This indicates that interface strain induced degradation would be more pronounced for T_{ox} less than 2 nm. In addition, the thickness dependence of E_a corroborates excellently (except the data points in the circle region) with the interfacial strain indicating a strong link between them. Since the extracted NBTI E_a is very sensitive to gate oxide processing conditions (e.g. nitridation), therefore, we consider that the E_a data points in the circle region would be further reduced as a result of the influence of nitridation, in addition to the influence of interfacial strain. This is plausible, as nitrogen has been observed to lower the E_a , as demonstrated in Chapter Three. Hence, we can thus disregard the data points in the circle region and obtain a linear correlation between the interfacial strain and NBTI E_a as shown in Fig. 5.3(b). Finally, we speculate that this linear relationship shows Si-H bond weakening and more strained Si-O-Si bond formation with increasing strain. Both effects reduce the barrier for NBTI reaction.

Figure 5.3: (a) Gate dielectric thickness T_{ox} dependence on NBTI E_a and interfacial strain; (b) Correlation between interfacial strain and NBTI E_a (T_{ox} dependence of interfacial strain is re-plotted using the data from Ref 154).

5.2.4 Discussion

The atomic model proposed in Chapter Four is not sufficient to account for the minimization of NBTI by ISSG and the width dependence of NBTI. Moreover, from all the previous experimental observations, it is apparent that interfacial strain plays a significant role in NBTI. In order to provide a satisfactory explanation, the interfacial strain or stress effect on NBTI has to be taken into account, since there is a strong link between the interfacial strain/stress and NBTI. In addition, the gate dielectric thickness dependence of NBTI E_a provides strong evidence that an increase in interfacial strain reduces NBTI E_a . Thus, although this is not direct evidence, it supports the hypothesis in Chapter Three that the decrease in NBTI E_a with increasing nitrogen concentration is related to interfacial strain. Intuitively, one can relate the interfacial strain/stress to the weakening of interfacial property or increase of defect states, which in turn leads to deteriorate NBTI. We term this as strain-weaken NBTI. On the other hand, although interfacial strain can satisfactory explain the experimental results, it should be noted that the concentration of sub-oxide or sub-stoichiometric oxide increases proportionally with interfacial strain [154], thus, it is important to decouple the effect of interfacial strain and sub-oxide to provide further insight into NBTI.

Despite the importance of the transition layer at the interface, there is no study available to examine the impact of transition layer on NBTI-induced degradation. This is probably because it is difficult to verify experimentally that the strained-SiO₂ or non-stoichiometric SiO₂ network degrades NBTI. Although it is difficult to study experimentally, one can address the problem from theoretical calculation e.g. First-Principles Calculations. To establish a direct link between the interfacial strain and NBTI, we shall re-examine and take a closer look at the atomic model proposed in

Chapter Four. In this scenario, we look into the bond angles of the structures involved in NBTI reaction. This is because bond angle is a direct measure of strain in a film. An increase in the compressive strain will decrease the bond angle value from its original value in a completely strain-free structure. In contrast, tensile strain will have an opposite effect. Figure 5.4 shows the bond angles for Si-H bond and Si-O-Si bond before and after NBTI reaction, respectively. As seen, the equilibrium bond angle for Si-O-Si is 138° after geometry optimization, which reasonably agrees with the strain-free Si-O-Si bond angle of 144° . This indicates yet another validation for the model used.

Figure 5.4: Bond angles for Si-H bond and Si-O-Si bond before and after NBTI reaction, respectively. The angles are obtained after the geometry is optimized for each model.

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As can be observed from Fig. 5.4, the bond angle of the Si-Si-Si bond is increased from 110.86° to 116.04° , i.e. $\sim 5\%$ change after Si-H bond dissociation. Conversely, the bond angle of Si-O-Si is decreased from the 138.03° to 127.33° , i.e. $\sim 8\%$ change after trapping the hydrogen released from the Si-H bond. We also obtain a similar bond angle reduction of approximately 6% for the Si-N-Si bond after the capture of released hydrogen species in nitrided film. The variation of bond angles before and after NBTI should be interpreted as follows. If these non-equilibrium bond angles (116.04° of Si-Si-Si bond or 127.33° of Si-O-Si bond) exist in the Si/SiO₂ interface, the NBTI reaction energy barrier will lower than that of the equilibrium structures. This is possible, as a matter of fact that these non-equilibrium angles only exist in the presence of local network strain in the transition layer of SiO₂. This analysis also coincides with the previous finding that NBTI occur mostly at/near Si/SiO₂ interface. It further confirms the importance of interfacial strain/stress on NBTI as shown in previous experimental demonstration. Although the effect of interfacial strain has been elucidated, an understanding of NBTI dependence on various interfacial topologies as a result of stoichiometric oxide is still largely illusive. However, the effect of interfacial strain is only practically known, a detailed understanding is still lacking. In particular, the question on how relaxation of interfacial strain improves the NBTI immunity in atomic level remains unsolved.

5.3 Impact of interfacial strain on NBTI

To further understand the effect of interfacial strain on NBTI, we extend the atomic model to incorporate the strain effect. According to the model proposed in Chapter Four, the NBTI reaction could be described by hydrogen-originated hole trapping. The first step of the reaction is Si-H bond dissociation followed by the diffusion and trapping of the released hydrogen species. Hence, we concentrate on the impact of interfacial strain on the Si-H bond dissociation process and the trapping of released hydrogen species. Since any variation of bond angle is a good indication of interfacial strain, we should first obtain the equilibrium bond angle for the precursor structures involved in NBTI reaction, for the study of NBTI dependence on strain. Subsequently, the bond angle is fixed at preset non-equilibrium values ranging from $\pm 60^\circ$ from its equilibrium bond angle and the geometry is reoptimized for all other degrees of freedom. The total energy calculation models and procedures are similar to that described in Chapter Four. Note that the bond angle variation of $\pm 60^\circ$ is justifiable and practical because it has been demonstrated that Si-O-Si bond angle distribution at Si/SiO₂ interface can be varied from 120° to 180° [34,145], which vary as much as 40° from the ideal bond angle, 144° .

5.3.1 Effect of strain on Si-H dissociation process

Fig. 5.4 depicts the equilibrium bond angle of the Si₃-Si-H structure. Specifically, the equilibrium geometry for the $\angle\text{Si-Si-H}$ and $\angle\text{Si-Si-Si}$ in this case is 108° and 110.86° , respectively. We will vary these bond angles to elucidate the effect of strain on the Si-H bond dissociation process. The interfacial strain-induced deviation of $\angle\text{Si-Si-H}$ and $\angle\text{Si-Si-Si}$ is varied from 48° to 168° and 50° to 150° , respectively. After which, the geometry

is optimized for all other degrees of freedom except the preset distorted angle. Finally, the Si-H bond energy E_B is calculated by computing the total energy of a H atom and the remaining fully relaxed doublet molecule cluster, and subtracting it from the total energy of the respective Si-H cluster. This difference in energy must be accounted for by the Si-H bond, which is present in the product but not in the reactants.

Figure 5.5: Plots of Si-H bond energies relative to its equilibrium value as a function of the change of bond angle for Si-Si-H and Si-Si-Si bond. The bond energy values are obtained from the first-principles calculations.

The Si-H bond energy relative to its equilibrium value, is plotted as a function of the change in the bond angle of Si-Si-H and Si-Si-Si bond, as shown in Fig. 5.5. Figure 5.5 has a few interesting features. Firstly, the bond energy difference reduces as the bond angles for Si-Si-H and Si-Si-Si deviate from their equilibrium values, indicating a gradually weaker Si-H bond. This result provides strong evidence that the Si-H bond

strength is weakening with increasing interfacial strain. In addition, it is consistent with the recently proposed generalized simple thermal mode [56], [112] for the Si-H dissociation that the spread of Si-H bond dissociation energy increases with increasing interfacial strain. This finding also provides confirmation for a recent experimental study, which reported a direct correlation between oxide reliability and physical stress at the interface [170]. This weakening effect is independent of the type of stress, i.e. whether it is compressive or tensile stress. A closer examination on the data reveals that bond energy degradation is not exactly symmetrical between compressive and tensile stress. The former contributes slightly larger bond energy lowering than the later for a similar change of bond angle. This finding is disturbing because SiO₂ film on Si substrate is known to have compressive stress at the transition layer as shown in Fig. 5.3. Another disturbing observation is that the deviation of the bond energy difference, associated with a shrinking the bond angle, is larger for $\angle\text{Si-Si-Si}$ than for $\angle\text{Si-Si-H}$. This has strong implication on the mechanical stress imposed on the active channel region. In this scenario, the STI-induced compressive stress may distort the $\angle\text{Si-Si-Si}$ that resides at the active channel side, hence weakening the Si-H bond eventually. This suggests that there is a close link between NBTI and STI-induced stress and consistent with the observed width-dependence of NBTI effect in Fig. 5.2.

Lowering of the Si-H bond strength due to increasing strain or stress (that is deviation of bond angle) can be attributed to an increase in the potential energy of the disturbed Si-H bond state, which subsequently forms a weaker bond. Furthermore, the interpretation of this result should not be limited to strain-weaken NBTI effect but it can also be applied to other reliability issues, such as width-dependence of hot carrier effect and improved TDDB lifetime of steam oxide over dry oxide.

5.3.2 Effect of strain on hydrogen-originated hole trapping reaction

To further investigate the effect of strain on NBTI, we vary the $\angle\text{Si-O-Si}$ and $\angle\text{Si-N-Si}$ for pure SiO_2 and nitrided oxide. We then perform the calculation for hydrogen-originated hole trapping reaction, as described in Eqs. 4.6 and 4.7 for pure SiO_2 and nitrided oxide, respectively. Figure 5.6 shows the NBTI reaction energies relative to its equilibrium value, plotted as a function of the change in bond angle for the Si-O-Si and the Si-N-Si bond. To consolidate the strain effect on the bridging atom, we shall not consider the strain effect on Si-H bond to simplify the interpretation. From Fig 5.6, it is found that the NBTI reaction energy is reduced in both SiO_2 and nitrided oxide when $\angle\text{Si-O-Si}$ and $\angle\text{Si-N-Si}$ deviates from its equilibrium value is inevitable. The reduction of reaction energy means NBTI can happen more easily. This provides another evidence that NBTI can be further deteriorated in the presence of interfacial strain at the positive charge trapping site, be it compressive or tensile stress. Similar to the case of Si-H bond, compressive stress at the trapping site seems to have larger impact on the NBTI reaction. This finding poses another alarming signal to the importance of relaxing the compressive stress in the transition layer. Furthermore, the reduction in NBTI reaction energy is larger in nitrided oxide, as compared to pure SiO_2 , for a similar change in the bond angle. This means that the nitrided oxide is more susceptible to interface strain as compared to pure SiO_2 in term of NBTI degradation. This could cause the nitrogen- weaken NBTI effect to be more pronounced in the presence of strained structures at the interface. In this case, the strained structures refer to strained Si-O-Si and Si-N-Si bond at the Si/ SiO_2 and Si/ SiO_xN_y interface respectively. Therefore, combining the study of strain effect on Si-H bond strength and Si-O-Si/Si-N-Si bond, it provides further support to the hypothesis in Chapter Three that the decrease of NBTI E_a is also related to the increasing interfacial

strain, as well as nitrogen-induced reaction energy lowering presented in Chapter Four. In this scenario, excessive nitrogen incorporation is assumed to increase the interfacial strain [70],[123],[124]. This speculation is plausible and in agreement with a recent molecular orbital calculations that NO nitridation increases the interfacial strain [113]. Furthermore, the same assumption has been proposed to explain the weakening of Si-H bond in highly nitrided oxide [123],[124]. Putting aside the speculation, Fig. 5.6 clearly indicates that the strain-weaken NBTI effect would be more severe in nitrided oxide than in pure oxide, for a similar amount of interfacial strain. Therefore, it is essential to relieve the strain-weaken NBTI degradation. Future devices should be designed with consideration to reduce the stress and one potential solution is using steam oxide like ISSG.

Figure 5.6: Plots of NBTI reaction energies relative to its equilibrium value as a function of the change of bond angle for Si-O-Si and Si-N-Si for pure SiO₂ and nitrided-oxide, respectively.

5.4 Impact of oxide stoichiometry on NBTI

We have demonstrated the impact of strain on NBTI. Next, the impact of oxide stoichiometry on NBTI is addressed. Previously in Chapter Four, the properties of the model Si/SiO₂ interface are based on an abrupt Si/SiO₂ interface containing the minimum transition region required to accommodate the structural change from bulk Si to bulk SiO₂. To be fully consistent with core-level photoelectron spectroscopy measurements of experimental Si/SiO₂ interfaces, however, all three partial oxidation states of Si should be present in the transition region in comparable amounts [143],[171]. The partial oxidation state are denoted as Si¹⁺, Si²⁺ and Si³⁺ which means Si atoms have one, two, and three nearest-neighbor oxygen atoms, respectively. It is therefore important to understand the impact of suboxides bonding on NBTI reaction in particularly Si-H dissociation and released hydrogen trapping at bridging O and N atom.

5.4.1 Effect of oxide stoichiometry on Si-H dissociation process

In studying on the dependence of Si-H bond dissociation on oxide stoichiometry, we use the seven atomic models shown in Fig. 5.7 to represent the various possible configurations of Si-H bond at the Si/SiO₂ and Si/SiO_xN_y interfaces. As shown in Fig. 5.7, structure (i) comprises a Si-H bond with a backbone of three Si atoms; for structures (ii) to (iv), the number of O, as first-nearest-neighbor (1st-NN) to Si-H is increased from one to three to depict the influence of different partial oxidation states. Since all bonds remain fully saturated, the interface remains electrically ideal, as required. The process of increasing O atoms from the transition region is expected to be a fairly general prescription for generating suboxide states near the Si interface. On the other hand, in the Si/SiO_xN_y structures, an N atom substitutes an O atom as the 1st-NN to depict the

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influence of different partial nitridation states. After geometry optimization, the bond length for various structures is in good agreement with that reported in the literature suggesting that our relaxed models give a good representation of the localized structures at the interfaces.

Si/ SiO ₂
Si-H ΔE_B	(i) Si ⁰⁺ = 0.0	(ii) Si ¹⁺ = 0.10	(iii) Si ²⁺ = 0.29	(iv) Si ³⁺ = 0.62
Si/ SiO _x N _y
Si-H ΔE_B	NA	(v) Si ¹⁺ = -0.02	(vi) Si ²⁺ = 0.21	(vii) Si ³⁺ = 0.54

Figure 5.7: Various possible Si-H cluster models at Si/SiO₂ and Si/SiO_xN_y interface to denote different partial oxidation or nitridation states. The bond energy differences (ΔE_B) for Si-H are obtained from first-principles calculation. The calculated bond energies are then compared with structure (i). The unit for energy is in eV.

After geometry optimization, the Si-H bond energy, E_B , for these structures are calculated and compared in Fig. 5.7. At the Si/SiO₂ interface, the Si-H bond energies are

0.10, 0.29 and 0.62 eV higher in structure (ii), (iii) and (iv), respectively, as compared to that of structure (i). This indicates that the Si-H bond becomes stronger as the number of O as 1st-NN increases from one to three. In other words, the Si-H bond in SiO_x ($0 \leq x \leq 2$) becomes stronger as x increases. Therefore, the Si-H bond is weakest at the Si-rich interface, while it is strongest in the stoichiometric oxide. Interestingly, when an O atom is replaced by a N atom at Si/SiO_xN_y interface, the Si-H bond energy increases with the number of N atoms, indicating that the bond becomes stronger also. More importantly, E_B slightly deteriorates by 0.08 to 0.12 eV following replacement of O atoms by N atoms.

The Si-H bond energy comprises of molecular covalent single-bond energy and ionic contribution due to the difference in the electronegativity of the Si and H atoms. The greater the electronegativity difference, the greater the ionic contribution of the particular bond, and hence a stronger bond. Therefore, the variation in Si-H bond energy can be explained in terms of electronegativity of the neighboring atoms (the electronegativity of Si, N and O atoms are 0.18, 0.3 and 0.35, respectively). In this scenario, the neighboring O atoms have a larger ionic contribution to the total bonding energy of the Si-H bond as compared to the neighboring Si atoms. As such, as shown in Fig.5.7, structure (i) has the lowest E_B while structure (iv) has the highest E_B, suggesting that the Si-H bond is weakest in the Si side of the interface but strongest in the bulk stoichiometric oxide. The above situation also suggests that replacing O by N would reduce E_B, as shown in Fig.5.7 for the Si/SiO_xN_y interface (structures (v) - (vii)). Note that E_B for structure (v) is even slightly lower than that for structure (i). As a practical Si/SiO_xN_y interface is likely to be dominated by structure (v), this has the important implication that Si-H bond at the Si/SiO_xN_y interface is slightly weaker than that at the Si/SiO₂ interface.

5.4.2 Effect of oxide stoichiometry on hydrogen-originated hole trapping reaction

To investigate the oxide stoichiometry on hydrogen-originated hole trapping reaction as described in Eqs. 4.6 and 4.7, we use the eight atomic models shown in Fig. 5.8 to represent various possible configurations of bridging atom at Si/SiO₂ and Si/SiO_xN_y interfaces. As shown in Fig. 5.8, structure (i) is a Si-O-Si bond with the backbone of three Si atoms; for structures (ii) to (iv), the number of O as 1st-NN to Si-O-Si increases from one to three to depict the influence of different partial oxidation state. Similar bonding configurations are applied to interfacial models of Si/SiO_xN_y interface. It should be noted that nitrogen surrounding the Si atom is considered to increase the oxidation state for the interface. In addition, the bond length for various structures is in good agreement with other literatures validating our relaxed models as a good representation of the localized structures at the interfaces.

After geometry optimization, the NBTI reaction energy for these structures are calculated and compared as shown in Fig. 5.9. In this scenario we do not consider the stoichiometry effect on Si-H bond to simplify the interpretation and the released hydrogen is originated from Si₃Si-H bond for all the eight models. Unlike interfacial strain, it is evidently shown in the Fig. 5.9 that reaction energy of hydrogen-originated hole trapping reaction at Si/SiO₂ and Si/SiO_xN_y interface is independent of stoichiometric oxide. This means that the released hydrogen trapping reaction is independent of stoichiometric oxide as well but the nitrogen-enhancement remains unaffected in these structures. The independent of NBTI on stoichiometric oxide is probably due to negligible alteration of electron density distribution around the trapping center. This is because as demonstrated in Chapter Four that atomic charge around the atom can affect the NBTI significantly.

Figure 5.8: Various possible interfacial models at Si/SiO₂ and Si/SiO_xN_y interface to denote the different partial oxidation or nitridation states. The atom in the box represents the trapping center for released hydrogen species.

Figure 5.9: Plots of NBTI reaction energies relative to that of structure (i) from Fig. 5.7 as a function different partial oxidation state.

5.5 Chapter summary

We experimentally demonstrated that the transition layer near the Si/SiO₂ interface might have strong impact on the NBTI degradation of ultra-thin gate oxide, i.e. the relaxation of the strain within 1nm thick from Si/SiO₂ interface is proposed to minimize the NBTI degradation. The experimental hypothesis is confirmed by the theoretical study using First-Principles calculation. The calculations have shown that the bond strength of NBTI precursor, that is Si-H, is strongly weakened by the interfacial strain. Furthermore, the reaction energy of hydrogen-originated hole trapping reaction is lowered by the interfacial strain. Although both compressive stress and tensile stress enhance NBTI, the former seems to have larger influence than the later one. This is disturbing, as the compressive stress is always present at Si/SiO₂ interface. Conversely, the effect of stoichiometry oxide on NBTI is less problematic. It is observed that Si-H bond strength is weaker at when reside at sub-stoichiometric oxide than that at stoichiometric oxide. In addition, it is slightly weaker at Si/SiO_xN_y interface than at Si/SiO₂ interface. Unlike interfacial strain, the reaction energy of hydrogen-originated hole trapping reaction is not affected by stoichiometric oxide.

In short, this chapter reveals that the controlling of the strain layer property within 1nm thick is extremely important for future ultra-thin gate oxides with high reliability in sub-65 nm ULSI technology. Therefore, relaxation of the strained-layer is more requisite issue to improve the reliability and to realize the aggressive scaling. Furthermore, combining the results from previous Chapters and this Chapter, we further conclude that the nitrogen-worsen NBTI effect cannot be simply explained by a single or double factor. As demonstrated, nitrogen at Si/SiO_xN_y has multiple negative effects: (1) create more NBTI precursors (that is more N and Si-H bond); (2) lowering the NBTI reaction energy;

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(3) slightly weakening of Si-H bond strength and finally, (4) increases the susceptibility against strain-weaken NBTI effect.

CHAPTER SIX

Dynamic NBTI in PMOS transistor

This chapter focuses on an important aspect of NBTI in PMOS transistor namely dynamics NBTI, and aims to develop an efficient and reasonably accurate lifetime model to facilitate dynamic lifetime extraction from the static measurement. This is accomplished through a comprehensive comparative study on the effect of dynamic NBTI stress on time, oxide field and temperature dependence with static NBTI. In addition, the frequency and duty cycle on device degradation is discussed. Discussion will also be focused on the characteristic of the annealing effect in DNBTI and its implication to the lifetime of pMOSFETs. The mechanism of the annealing effect is proposed to be the reverse reaction of NBTI. Consequently, another comparison on the three types of digital waveforms is carried out and their impact on degradation is discussed.

6.1 Introduction

The NBTI degradation of pMOSFET devices has been widely recognized as a limiting factor for the scaling down of circuit dimensions. However, little interest has so far been devoted to the study of transistor degradation under realistic bias conditions, reproducing the dynamic operation cycles experienced by the devices during their lifetime. Much works, as mentioned in previous chapter, has been devoted, on the contrary, to the prediction models based on static stress bias. As a result of these studies, it is generally believed that, regardless of the real dynamic operation cycles, static stress operation, coupled to the choice of proper monitor parameters (typically threshold voltage, transconductance, or drain current), may give reliable predictions of the device lifetime. Therefore, relatively little information exists on NBTI under dynamic stress condition. This is certainly due to the difficulties in conducting these tests and also due to the wide belief that static stress underestimates the lifetime of oxides subjected to dynamics stress conditions. The lack of NBTI wear out data under dynamic conditions was pointed out and the need for it was emphasized recently [11].

6.2 Experimental setup

P⁺-gate pMOSFET's with $W \times L = 10 \times 0.12 \mu\text{m}^2$ were fabricated using standard dual-gate CMOS technology. The details of the fabrication processes can be found in the Chapter 3. Static NBTI (SNBTI) stress was applied to a device at low constant negative gate bias (-1.8 to -3 V) under 125 °C. While dynamic NBTI (DNBTI) stress was applied by using a pulse generator. The DNBTI is tested under three different dynamic modes namely: (a) unipolar [DNBTI_{uni}], (b) bipolar [DNBTI_{bi}] and (c) dynamic operating mode of pMOSFET in an inverter circuit [DNBTI_{inv}], as depicted in Fig. 6.1. Note that DNBTI_{inv} stress condition is to simulate the operating condition of pMOSFET in a CMOS inverter. The pulses to both the gate (V_g) and one of the diffusion regions (V_d) were from the same pulse generator but were out of phase such that the diffusion was at ground potential while the gate was high (i.e. negative bias) and vice versa. In this inverter-like waveform, both V_g and V_d are of the same magnitude. The setup configuration is shown in Fig. 6.2. The rise/fall time of the pulses were set to be 5 % of the period. The output of the pulse generator is connected to a 50-Ohm resistor for output impedance matching that keeps the shape of the waveform properly. The stress was interrupted at a predetermined period to measure the threshold voltage and the drain current. The device lifetime is defined as the time needed for a threshold voltage shift (ΔV_{th}) of 30 mV.

Figure 6.1: Definition of different dynamic stress waveforms: (a) unipolar, (b) bipolar, and (c) dynamic operation mode of pMOSFET in an inverter.

Figure 6.2: Setup configuration of pMOSFET under inverter-like waveform stress.

6.3 Mechanism of recovery phenomena in DNBTI

6.3.1 Behavior of transistor performance under DNBTI and their correlation study

Figures 6.3(a)-(c) compare the behaviors of ΔV_{th} , $\Delta G_{m,peak}$ and ΔI_{Dsat} under static and dynamic NBTI stress. For DNBTI, the gate pulse alternated between -2.2 V and 0 V with a period of 2000 s. It is evidently shown that the device degradation is recovered partially during $V_{g,top} = 0$ V, resulting in a smaller overall degradation compared to static stress. As can be seen from the figure that the ΔV_{th} , $\Delta G_{m,peak}$ and ΔI_{Dsat} are increasing and decreasing simultaneously during the ON-OFF-ON sequence. Therefore, the degradation of V_{th} , $G_{m,peak}$ and I_{Dsat} are probably due to the same origin of defects generation i.e. interface trap and positive oxide charge generation. This re-confirms the correlation study of Figs. 3.9 and 3.10 in Chapter Three that reveals the common origin responsible for V_{th} , $G_{m,peak}$ and I_{Dsat} .

A closer look at Fig. 6.3 reveals DNBTI exhibiting smaller overall degradation compared to static stress, but degradation is still increasing gradually despite the annealing effect. To evaluate the passivation quantitatively, we define a parameter called defect passivation fraction (DPF) as follow,

$$DPF = \frac{(|V_{th,passivated}| - |V_{th,stressed}|)}{(|V_{th,stressed}| - |V_{th,fresh}|)} \quad (6.1)$$

where $V_{th,stressed}$ is V_{th} after 1000 s of NBTI stress, $V_{th,passivated}$ is V_{th} after 1000 s of annealing (i.e. $V_{th,fresh} \rightarrow 1000$ s NBTI $\rightarrow V_{th,stressed} \rightarrow 1000$ s Anneal $\rightarrow V_{th,passivated}$). Based on the five stress/anneal cycles in Fig. 6.3(a), we re-plotted the DPF of each cycle and present in Fig. 6.4. In Fig. 6.4, after 1st stress/anneal cycle, about 35 % of the defects is being annealed.

Figure 6.3: Time dependence of (a) ΔV_{th} ; (b) $\Delta G_{m,peak}$ and (c) ΔI_{Dsat} under static and dynamic NBTI conditions [unipolar waveform] .

After another four consecutive cycles, the defect recovery is linearly reduced from 35 to 22 %, implying a growing number of permanent damages that are unable to be annealed out even when NBTI stress is removed.

Figure 6.4: Plot of DPF as a function of the number of stress/anneal cycle.

To further understand the behavior of the annealing during OFF sequence, the results in Fig. 6.3 are re-plotted as a $\Delta G_{m,peak}$ vs ΔV_{th} and ΔI_{Dsat} vs ΔV_{th} characteristic in Figs. 6.5(a) and 6.5(b) respectively. One can observe that $\Delta G_{m,peak}$ and ΔI_{Dsat} increase linearly with ΔV_{th} under the NBTI stress. More importantly, after removing NBTI stress, $\Delta G_{m,peak}$, ΔV_{th} and ΔI_{Dsat} begin to decrease with keeping the linearity. It is worth mentioning that the decreasing $\Delta G_{m,peak}$ suggests that NBTI-induced interface traps are being annealed out partially. Looking more closely at Fig. 6.5, it is noticed that the linear relationship is excellently fitted from the origin.

Figure 6.5: Correlation between (a) $\Delta G_{m,peak}$ and ΔV_{th} ; and (b) ΔI_{Dsat} and ΔV_{th} for NBTI stress and annealing. The data are obtained from Fig. 6.3.

The origin-fitted linear relationship in Fig. 6.5 provides strong evidence on NBTI recovery in which both NBTI-induced N_{it} and N_{ox} are responsible for the recovery. This can be explained by following reasons. Firstly, in Chapters Three and Four has demonstrated that both N_{it} and N_{ox} charges increase proportionally with respect to NBTI stress, hence recovery follows the same linearity with degradation can be attributed to the passivation of both N_{it} and N_{ox} generated during NBTI stress. Secondly, if the recovery is due to other passivation mechanism, then one should not obtain a similar linearity with degradation as illustrated in Fig. 6.6. If the recovery is dominated by N_{ox} passivation then one should expect a smaller slope than that of degradation based on Fig. 6.6. On the other hand, if recovery dominated by N_{it} passivation then the slope of recovery should be higher than that of degradation. The most probable explanation for the same linearity for both recovery and degradation is both NBTI-induced N_{it} and N_{ox} are passivated during the annealing phase.

Figure 6.6: Illustration of various recovery paths during annealing phase. Square represents the NBTI-induced degradation; Circle means annealing-induced recovery.

6.3.2 Behavior of interface trap and positive oxide charge under DNBTI

To confirm the above analysis, the direct-current current-voltage (DCIV) is used to study the behavior of the recovery and the results are shown in Fig. 6.7. DCIV is performed at the stress temperature in order to mitigate the unwanted annealing effect on degradation during cooling down of the chuck. As observed from Fig. 6.7 (a), the peak of I_{DCIV} is increased after NBTI, as expected, however when stress is removed, the peak of I_{DCIV} is reduced to a lower level of N_{it} with time. Since the peak of I_{DCIV} is proportional to the interface trap density (for detail of DCIV, refer to Chp. 3, pg. 48), this result indicates that NBTI-induced N_{it} is annealed out when the stress is removed and such annealing increases with time. Figure 6.7(b) shows the time dependence of ΔI_{DCIV} under DNBTI. Gate pulse is alternated between -2.2 V and 0 V with a period of 2000 s. Similar behavior is observed in both Figs 6.3 and 6.7 confirm the improvement is due to the passivation of N_{it} generated during the NBTI stress. This finding is consistent with previous studies [31], [32] that N_{it} created during NBTI can be removed partially. Hence, if a transistor that has been exposed to NBTI at a certain stress temperature and remains at that temperature with the gate grounded, the number of N_{it} should slowly decrease to a new level of N_{it} .

Figure 6.8 demonstrates the ΔV_{MG} as a function of NBTI stress and annealing. It is found that NBTI-induced ΔV_{MG} is reduced when stress is removed. As cited earlier in Chapter Three, the ΔV_{MG} is proportional to the positive oxide charge density at the interface (for detail of ΔV_{MG} , refer to Chp. 3, pg. 49). Thus, this experiment confirms that N_{ox} can be annealed when NBTI stress is removed. Moreover, comparing Figs. 6.3, 6.7 and 6.8, one can conclude that the reduction of ΔV_{th} is attributed to annealing of NBTI-induced N_{it} and N_{ox} .

Figure 6.7: (a) Behavior of DCIV current during and after NBTI stress. The arrow depicts the direction of peak current increases and reduces, respectively; (b) the time dependence of ΔI_{DCIV} for NBTI stress and annealing.

Figure 6.8: Time dependence of mid-gap voltage shift ΔV_{MG} for NBTI stress and annealing.

As shown in Fig. 6.8, the ΔV_{MG} variations are almost perfectly reversible when a suitable detrapping phase (i.e. gate is grounded at stress temperature) is performed. This behavior is fully consistent with trapping and detrapping dynamics of positive charge [175],[176]. When the results in Figs. 6.7 and 6.8 are re-plotted as a ΔI_{DCIV} vs ΔV_{th} and ΔV_{MG} vs ΔV_{th} characteristic in Figs. 6.9(a) and 6.9(b), it can be clearly seen that both ΔI_{DCIV} and ΔV_{MG} increase linearly with ΔV_{th} under the NBTI stress. More notably, after the NBTI stress is removed, ΔI_{DCIV} , ΔV_{MG} and ΔV_{th} begin to decrease maintaining the same linearity. These results show that both NBTI-induced N_{it} and N_{ox} are annealed out partially when the stress is removed and provide direct evident for the analysis in section 6.3.1.

Figure 6.9: Correlation study of (a) ΔI_{DCIV} vs ΔV_{th} and (b) ΔV_{MG} vs. ΔV_{th} for NBTI degradation and annealing phase. The data are obtained from Figs. 6.7 and 6.8.

6.3.3 Effect of the positive gate voltage on recovery phenomena

It has been known that applying a positive gate bias consecutively to a negative bias stress could neutralize both trapped holes and/or positively charged slow state [174]. Therefore, we study the effect of positive gate bias on this recovery phenomenon and results are depicted in Fig. 6.10. It is observed that passivation rate is electric field dependence, i.e. large the field applied, the more rapid the passivation. The strong field dependence suggests that charged species (e.g. H^+ or OH^+) are likely to be generated during NBTI stress. This is not surprising, as discussed in the Chapters Three and Four; positive oxide charges ($Si-OH^+-Si$ for pure SiO_2 and $Si-NH^+-Si$ for SiO_xN_y) are generated during NBTI. Therefore, intuitively higher positive gate oxide field could neutralize more hydrogen-originated positive oxide charges.

Figure 6.10: Dependence of various positive gate biases on the recovery of ΔV_{th} .

Figure 6.11: Effect of positive gate bias (a) $+0.5 V$ and (b) $+1 V$ on correlation study of $\Delta G_{m,peak}$ vs ΔV_{th} for NBTI degradation and annealing phase. The data are obtained from Figs. 6.10.

Figure 6.11 demonstrates the effect of positive gate bias on correlation study of $\Delta G_{m,peak}$ vs ΔV_{th} for NBTI degradation and annealing phase. Several features worth to take note from this figure. Firstly, there is no marked differences are observed for the recovery's slope (i.e. recovery path) and the degradation's slope for both biases. This is unexpected because when higher gate voltage is applied, higher amount of positive oxide charge should get neutralized through detrapping. According to Fig. 6.5, if neutralization of positive oxide charge is dominating in recovery process when positive gate bias is applied during T_{off} , one should anticipate smaller annealing slope than that of degradation in $\Delta G_{m,peak}$ vs ΔV_{th} plot and the slope should be even smaller as positive bias goes higher. Secondly, through careful comparison of Figs. 6.11(a) and 6.11(b), one can see higher positive gate bias enhances the recovery (as indicated by the arrow in respective figures). Based on the analysis in section 6.3.2, the unique feature of similar linearity for both degradation and recovery with origin-fitted indicates both N_{it} and N_{ox} generated during NBTI being responsible for the recovery. The effect of positive gate bias on recovery can be interpreted by considering the detrapping of hydrogen-originated trapped hole (i.e. $\text{Si-OH}^+-\text{Si}$ for pure SiO_2 and $\text{Si-NH}^+-\text{Si}$ for SiO_xN_y^+). In this scenario, higher detrapping of OH^+ and NH^+ release more hydrogen species, which can later involve in the passivation process of NBTI-induced interface traps. Consequently, one can deduce that when higher positive gate bias is applied, more N_{it} and N_{ox} generated during NBTI can get passivated.

6.3.4 Temperature dependence of ΔV_{th} during NBTI stress and annealing phase

The temperature dependence of ΔV_{th} during NBTI stress and annealing phase is depicted in Fig. 6.12. It is apparent from Fig. 6.12(a) that both degradation and recovery strongly depend on the temperature. The activation energies of the threshold voltage shift have been determined at the end of the NBTI stress i.e. point A in Figure 6.12(a), after the annealing (point B), and at the end of another cycle of NBTI (point C) as shown in the Figure 8. At the end of the NBTI stress (point A), the activation energy ($E_{[A]}$) is equal to 0.14 eV, in agreement with activation energy of point C ($E_{[C]} = 0.12$ eV) although its magnitude is slightly weaker. This corresponds to NBTI activation energy. After applying a 1000 s of annealing phase and as the threshold voltage shift is reduced, its activation energy (i.e. $E_{[B]}$) is then equal to 0.13 eV, similar to the activation energy of the NBTI (i.e. point A and C). This should be interpreted as the threshold voltage shift after the annealing phase is still depending on both the creation of interface traps and positive oxide charges although annealing can suppress both of them.

Consequently, the threshold voltage shift consisting of the difference of the threshold voltages before and after the annealing phase represents the contribution of both N_{it} and N_{ox} induced during the NBTI stress. Therefore, the activation energy ($E_{[A-B]}$) should be comparable with $E_{[A]}$ and indeed $E_{[A-B]}$ is found to be ~ 0.14 eV. This finding is significant because it compliments previous analysis that both interface trap and positive oxide charge are involved in NBTI degradation and annealing. In addition, it is in contrast to the previous report that annealing is mainly dominated by hole detrapping [177], this is because the observed $E_{[A-B]}$ shows noticeable temperature dependence unlike the insignificant temperature dependence observe experimentally for hole trapping [178].

Figure 6.12: (a) Temperature dependence of ΔV_{th} during NBTI stress and annealing phase and (b) Arrhenius plots for various phase of part (a).

6.3.5 Time dependence of ΔV_{th} during NBTI stress and annealing phase

To further understand the characteristic of ΔV_{th} during recovery phase, Figure 6.13 depicts the comparison of time dependence of ΔV_{th} during NBTI stress and annealing phase. Note that the annealing phase means the recovery of ΔV_{th} after an NBTI stress was stopped. Based on this figure, it is recognized that ΔV_{th} recovery also follows the power law with the exponent of 0.21, being the same as NBTI degradation. Two similar results have also been reported recently [172],[173] that the recovery of ΔV_{th} follows similar time dependence as NBTI degradation. This suggests that the recovery reaction is controlled by the diffusion of hydrogen species, which are consumed in the reverse reaction.

Figure 6.13: Time dependence of ΔV_{th} during NBTI stress and annealing phase. The time exponent value of 0.21 indicates that both ΔV_{th} are diffusion-controlled.

6.3.6 Effect of non-uniform oxide field and nitrogen on annealing phase

During the operation of a pMOSFET in a CMOS inverter, the applied gate bias (input signal) switches between “high” and “low” voltages, while the drain bias (output signal) alternates between “low” and “high” voltages, correspondingly. Therefore, to simulate a pMOSFET during the “low” phase in a CMOS inverter, a non-uniform electric field is applied during the annealing phase, that is, a negative drain bias is applied while other terminals are kept grounded. As shown in Fig. 6.14, the annealing effect is similar to that observed under the uniform electric field passivation. A closer look on the figure reveals that the ΔV_{th} during annealing is larger for higher stress field although the similar drain field is applied in both cases. This is attributed to large amount of defects generated during stress that can serve as precursors for the annealing phase.

Figure 6.14: Time dependence of ΔV_{th} for stress-anneal-stress cycle with various pair V_g and V_d . Note that a negative V_d is applied during annealing phase.

		V _g		
		-2.2	-2.6	-3.0
V _d	-3.0	0.55	-	0.41
	-2.6	-	0.47	-
	-2.2	0.50	-	0.36

Figure 6.15: Defect passivation fraction (DPF) under different pairs of V_g and V_d .

The larger ΔV_{th} during recovery do not necessary mean the defects can be easily annealed. To shed more light into this, DPF, in which ΔV_{th} during recovery is normalized to stress-induced ΔV_{th} as formulated in Eq 6.1, is used. The DPF for different pair of V_g and V_d is presented in Fig. 6.15. Consistent with the effect of positive gate bias in section 6.3.3, higher drain field promotes the passivation. However, increasing NBTI stress voltage, DPF is reduced despite the fact that larger ΔV_{th} during recovery as observed in Fig. 6.14. The reduced DPF means more permanent damage generated during higher stress voltage that cannot be annealed. Nevertheless, the non-uniform drain field annealing does not alter the recovery path as demonstrated in Fig. 6.16.

Figure 6.16: Correlation between (a) $\Delta G_{m,peak}$ and ΔV_{th} for NBTI stress and annealing. The data are obtained from Fig. 6.14.

To understand the effect of nitrogen on annealing the time dependence of ΔV_{th} under stress-annealing-stress cycle for various nitrided oxides is shown in the Fig. 6.17. It should be noted that a uniform normal oxide field is applied in this study. As expected, nitrogen-worsen NBTI effect appears for both stress periods. For comparison, two different kinds of pure SiO_2 grown by rapid thermal oxidation and in-situ steam generation are used. Consistent with study in Chapter Five, ISSG demonstrates highest immunity against NBTI stress, hence suggesting that it could be one the promising candidate for future technology in addition to plasma nitridation. Next, to understand the nitrogen effect on recovery mechanism, one should de-couple such nitrogen enhancement effect on ΔV_{th} during recovery phase. For this regard, DPF is used and the result is depicted in Fig. 6.18.

Figure 6.17: Time dependence of ΔV_{th} for stress-anneal-stress cycle with different nitrided oxides.

Figure 6.18: Plot of defects passivation fraction as a function of $+V_{g,top}$ for various nitrided oxides and pure oxides.

Several findings are obtained from Fig. 6.18. Firstly, larger $V_{g,top}$ enhances the recovery. Secondly, the defects in nitrided is more susceptible during recovery as compared to pure oxides for all $V_{g,top}$. In nitrided oxides, there are nearly 70 % of the total defects can be recovered as compared to that of 50 % in pure oxides when a +1 $V_{g,top}$ is applied during annealing phase. This behavior is linked to the difference in the trapping site for hydrogen in nitrided oxide and pure oxide. Chapter Four has shown that the released hydrogen would diffuse and trap by the nitrogen and oxygen for nitrided oxide and pure oxide, respectively. The nitrogen trapping center is more efficient than that of oxygen trapping center. Therefore, the migration energy for released hydrogen is smaller in nitrided oxide than that of pure SiO_2 . We shall discuss further in the next session about the migration energy.

6.3.7 Discussion on mechanism of recovery of NBTI-induced ΔV_{th}

In Chapter Three and Four, the reaction-diffusion (R-D) model has been proposed to explain the NBTI-induced degradation because it is consistent with the power-law dependence of NBTI degradation ($\Delta V_{th} \sim t^n$) during the ON state of the transistor (stress phase). In addition, the model adequately explains the one-to-one correspondence between the number of the N_{it} and the N_{ox} generated during the NBTI stress. According to the standard R-D model, NBTI degradation can be described as follow:

Also, it has been demonstrated that they can be generalized as the hydrogen-originated hole trapping reaction as show:

Firstly, the interface traps ($\text{Si} \bullet$) are generated from the dissociation of hydrogen terminated trivalent Si bonds (Si-H) by interaction with holes (h^+) in the Si inversion layer during NBTI stress. Then the released hydrogenated species (H^+) diffuse and are trapped near the oxide interface resulting in the positive oxide charges ($\text{Si-OH}^+-\text{Si}$ or $\text{Si-NH}^+-\text{Si}$). It should be noted that the diffusion process as described in reaction 6.2 controls the NBTI degradation. Another aspect about this model is that the released hydrogen species remain in the gate dielectrics as positive oxide charge and permanent damage

shall be created if the released hydrogen is escaped out of gate dielectric or trapped at the strain region near oxide interface.

Figures 6.7 and 6.8 have evidently shown that both N_{it} and N_{ox} are generated during NBTI stress and some of them disappeared after the NBTI stress is removed. More notably, the degradation and annealing consistently follow a similar linearity as shown in Figs. 6.5, 6.9, and 6.11. It is thus suggested that the reverse reaction of 6.5 and 6.6 occurred after NBTI stress is removed. This reverse reaction comprises of detrapping of hydrogen-originated positive oxide charge and reversal of Si-H dissociation process. In this scenario, when the gate bias polarity is reversed from the negative to positive or grounded, the channel inversion layer disappears and depletion layers are formed at source/drain. The breaking of Si-H bond stops due to lack of holes. At the same time, the reverse reaction occurs when the dissociated hydrogen, which remain in the gate dielectric as positive charges like OH^+ or NH^+ , diffuses back to the SiO_2/Si interface and passivate the Si dangling bonds, resulting in both ΔN_{it} and ΔN_{ox} reduction. The forward and reverse reaction of NBTI is illustrated in Fig. 6.19.

Figure 6.19: Illustration of forward and reverse reaction of NBTI at Si/SiO_2 interface.

During the recovery phase, H^+ is released from the loosely OH^+ and NH^+ bond at strain-free region in oxide. This is possible, as it has been demonstrated in Chapter Five that interfacial strain plays an important role in NBTI. In addition, we observed some NBTI-induced defects could be easily annealed; in particular, the annealing is very sensitive to the testing procedure like number of interruptions during stress cycle. For instance, for a total of 1000 s of NBTI stress if we interrupt the stress for ten times to measure transistor parameters like V_{th} and I_d ; the DPF would be around 60 %. However, if we interrupt the stress for four times, the DPF would be reduced to around 50 %. This is also consistent with previous studies [179],[180] that hydrogen-related structures can be thermally annealed easily. The anneal process is accompanied by the release of hydrogen species. The H^+ is then migrated back and passivate the interface trap. The migration path for H^+ is widely accepted as hopping mechanism, that is, hop from one O atom to adjacent O atom for SiO_2 and one N atom to adjacent N atom in the case of nitrated oxide, as illustrated in Fig. 6.20. Since the H^+ migration energy is smaller by 1.03 eV in nitrated oxide than that in SiO_2 (from Figure 4.4), hence, hydrogen species can reach more easily at Si/SiO_xN_y interface than at Si/SiO_2 . Therefore, more passivation of

Figure 6.20: Illustration of pathway for hydrogen ion in SiO_2 .

interface trap would occur by the adsorption of hydrogen at the dangling bond site [181] at Si/SiO_xN_y interface than that at Si/SiO₂ interface within the same time frame.

When H⁺ arrives at the interface and a dangling bond is present at the interface, H⁺ would be absorbed by dangling bond through Coulombic attraction. This can be proven by the atomic charge distribution calculation on the dangling bond structure as depicted in the Fig. 6.21. It is evidently shown that the Si dangling bond has a negatively charge center as predicted by three different atomic charge analysis, whereas positively charge is surrounding the remaining back-bonded Si atoms. Convincingly, the H⁺ would be absorbed at the dangling bond site if it reaches the site. During the absorption of hydrogen species at dangling bond, the Si-H⁺ will capture an electron from the Si substrate because the Fermi level is located near conduction band as the NBTI stress is removed. Therefore, applying a positive gate voltage during annealing is expected to enhance migration of OH⁺ or NH⁺ and release more hydrogen species for N_{it} passivation.

Interface cluster model for interface trap		Mulliken atomic charge analysis	Natural Population Analysis	Electrostatic potential based on Chirlian-Francel model
Si1	-0.1158e	-0.0416e	-0.1692e
	Si2	+0.1867e	+0.4354e	+0.7714e
	Si3	+0.1867e	+0.4356e	+0.3151e
	Si4	+0.1867e	+0.4355e	+0.6133e

Figure 6.21: Atomic charge distribution of the Si interface trap located at Si/SiO₂ interface.

The discussion has been focusing on H^+ as the diffusion species. Conversely, involving H atom in the reverse reaction is intuitively plausible, but this reaction process has several difficulties. Firstly, atomic hydrogen is highly chemically reactive in SiO_2 and therefore less stable than H^+ during transport [182]. So there are several competing reactions, including simple dimerization ($H + H = H_2$), which compete with it to become a more stable diffusion species both in the bulk of the oxide and near the Si/ SiO_2 interface. Secondly, it has also been argued theoretically that H^+ is a lower energy state than H in SiO_2 [183]-[187]. This suggests that, even if the atomic H does not react immediately, it would donate an electron and become H^+ again as soon as kinetically feasible. The key result that H remains positively charge in the oxide or at the interface is consistent with the known fact that H is a “negative-U” center in both Si and SiO_2 [184],[188]. Moreover, although two atomic H can dimerize and become a hydrogen molecule in turn diffuse to Si/ SiO_2 interface to passivate the interface trap but it is still insufficient to account for the dependence of recovery on positive gate voltage. Based on this analysis, we suggest that H^+ is the most probable diffusion species however; more experimental evidence is needed to confirm this suggestion.

Furthermore, as dictated by the model that both forward and reverse reactions are driven by the dissociated hydrogen diffusion, hence, both should have similar time dependence. This has been demonstrated in Fig. 6.13 that ΔV_{th} recovery follows the same power law dependence with NBTI-induced ΔV_{th} . Another interesting aspect related to this NBTI recovery model about the diffusion hydrogen species is that some of them remain in the gate dielectrics as positive oxide charge instead of the conventional belief that all hydrogen escape to gate electrode by dimerization during NBTI stress. Thus, one would anticipate higher amount of V_{th} recovery as a result of higher amount of hydrogen

remaining in gate dielectric that could diffuse back to the interface and contribute to annealing. This explains why one obtains a larger V_{th} recovery when NBTI-induced ΔV_{th} is large. Finally, it is clear that the reverse reaction is able to explain the experimental trends satisfactory. Besides, more appealing about this recovery model is that being consistent with the NBTI model described in Chapter Four, providing a further compliment and confirmation for our proposed NBTI model.

Additionally, at the time of completing this thesis, there have been quite a number of works on the recovery phenomenal in DNBTI [172],[173], [189]-[196]. However, only a few reported on the mechanism of recovery phenomenal. Some of them have attributed such a recovery to reverse reaction, but their discussion mainly focuses on the recovery of interface trap [172], [193]-[195], neglecting the association of interface trap recovery with that of positive oxide charge recovery. We believe such link is important, as demonstrated in this Chapter and Chapter Four, hydrogen species remain in as OH^+ , therefore, interface trap recovery mechanism is actually started off from these hydrogen trapping site. Furthermore, recovery in nitrided oxide is different from that of pure oxide as a result of the difference in term of OH^+ and NH^+ trapping center. On the other hand, a few has suggested that the recovery is dominated by the hole detrapping [177], however, this is inconsistent with the majority of work which observed interface trap is being recovered.

6.4 Waveform-dependence phenomenal model for DNBTI lifetime extraction

Presently, it has been recognized that static NBTI (SNBTI) model, which evaluates the pMOSFET degradation under DC NBTI test condition, can erroneously over-estimate the actual NBTI degradation for AC dynamic circuits even with frequency and duty cycle taken into consideration. This is because SNBTI model fails to account for the newly discovered NBTI recovery phenomenon [172],[190]-[192]. However, it remains an unresolved and challenging task to achieve a robust and accurate model for dynamic NBTI (DNBTI) since NBTI recovery rate is found to be sensitive to waveform frequency, duty cycle, voltage and temperature. In this session, we shall perform a detailed characterization of DNBTI for three types of digital waveforms, and formulate a waveform-dependent phenomenal model for DNBTI lifetime extraction of a pMOSFET in inverter operation.

6.4.1 Comparison of time, field and temperature dependence for SNBTI and DNBTI_{inv}

Figure 6.22 shows the comparison of ΔV_{th} between the SNBTI and DNBTI_{inv} stresses at 125 °C. For the DNBTI stress, inverter-like waveform with pulses of 10 KHz with 50 % duty cycle and $T_{rise}=T_{fall}= 5\%$ of period are employed. The experimental setup is illustrated in Fig. 6.22. The x-axis represents the total NBTI stress time (T_{on}) subjected to the devices. T_{on} is obtained by multiplying the total stress time by the duty cycle (for SNBTI, the duty cycle is 100%). Consistent with previous studies [172],[190], DNBTI exhibits smaller ΔV_{th} as compared to the SNBTI for a specified T_{on} . This is attributed to

Figure 6.22: Comparison of threshold voltage shift ΔV_{th} between the SNBTI and $DNBTI_{inv}$ stresses. The curves in represent the power-law fittings.

the re-passivation of both NBTI-induced interface states and positive oxide charges during T_{off} period for DNBTI stress, as discussed in earlier session. Furthermore, as shown in this Fig. 6.22, the stress time dependence of ΔV_{th} obeys a power law, i.e., $\Delta V_{th} = A.t^m$ where the prefactor A is a function of stress voltage, temperature and nitrogen content while m is the time exponent factor. The equations of the power-law fitting for various stress conditions are also shown in Fig. 6.22. It is found that the prefactor A increases with stress voltage but shows no difference between the static and dynamic stresses, indicating that the product of activation energy for the NBTI process and the field effects is the same for static and dynamic stresses. Furthermore, it shows no frequency dependence (Fig. 6.23a). On the other hand, the time exponent factor (m)

Figure 6.23: Parameters derived from time dependence of ΔV_{th} : (a) prefactor A versus stress gate voltage and (b) slope m versus frequency.

strongly depends on the stress methodology. A higher slope implies the device suffers higher degradation rate (for a given NBTI stress voltage and time) even though their initial characteristics may be the same. The value is significantly smaller for $\text{DNBTI}_{\text{inv}}$ compared to SNBTI, reflecting the fact that $\text{DNBTI}_{\text{inv}}$ is having a smaller NBTI-induced degradation. The time exponent factor is found to reduce with increasing frequency and obeys a logarithmic dependence on frequency (Fig. 6.23b).

To provide validation for expression A in Fig. 6.23(a), Fig 6.24 shows a comparison of the temperature dependence for SNBTI and $\text{DNBTI}_{\text{inv}}$. There is no apparent difference in the temperature effect between SNBTI and $\text{DNBTI}_{\text{inv}}$. This identical temperature dependent nature of the DNBTI and SNBTI is similar to that observed in comparable activation energies for AC and DC time-dependent dielectric breakdown study [197]. This data also validates the expression A and confirms that the product of field and temperature dependence of $\text{DNBTI}_{\text{inv}}$ is identical to SNBTI.

Figure 6.24: Comparison of temperature dependence of SNBTI and $\text{DNBTI}_{\text{inv}}$.

Based on the above results, if we are able to model the device lifetime-dependent on operating frequency, we should be able to extract the practical device lifetime through static measurement once calibration is completed since the field and temperature dependent remains unchanged for static and dynamic NBTI stress. Therefore, in the following sections, we shall focus on relationship between device lifetime and waveform frequency or duty cycle and consequently formulate a phenomenon waveform-dependent lifetime model for $\text{DNBTI}_{\text{inv}}$.

6.4.2 Duty cycle and frequency dependence

Figure 6.25 shows the relationship between the lifetime enhancement β (DNBTI lifetime/ SNBTI lifetime) and frequency for three different duty cycles. It has been shown previously that unipolar or bipolar dynamic stress increases the time-to-breakdown of SiO_2 thin films [198] and reduces the interface trap generation [197]. In addition, the observed dynamic lifetime enhancement occurred mainly for sufficiently high electric fields and large oxide thickness whereby charge trapping is significant [197]. It is generally believed that lifetime enhancement would be negligible small for direct tunneling oxide. However, in contrast to previous findings on dynamic FN tunneling stress, it is evident that the dynamic stress enhancement over static stress remains significant for DNBTI despite the facts that T_{ox} is merely 1.8 nm and the stress voltage is less than 3.5V (onset voltage of FN tunneling). Since the lifetime enhancement increases monotonically with smaller duty cycle and higher frequency, infer that shorter T_{on} and/or longer T_{off} pulses in DNBTI stress can result in more recovery and hence less overall degradation. From the result shown in Fig.6.25, one can formulate that the lifetime enhancement follows a power law dependence on frequency (*freq*):

$$\beta = K_1 \times freq^\gamma \quad (6.7)$$

where K_1 is a constant dependent on the duty cycle (its relationship with duty cycle is depicted in the inset of Fig. 6.25) but independent of frequency. We can then formulate an empirical DNBTI lifetime model (τ_{AC}) for any frequency and duty cycle (g) in terms of the SNBTI lifetime (τ_{DC}):

$$\tau_{AC} = K_2 \times \tau_{DC} \times freq^\gamma \times \exp(-\alpha \times g) \quad (6.8)$$

where γ , α and K_2 are constants independent of frequency, duty cycle, voltage and temperature, but sensitive to process technology. These constants can be obtained from the calibration of one-time DNBTI lifetime measurement for a small set of frequency/duty cycle matrix as shown in Fig. 6.25. The extracted parameters for γ , α and K_2 are 0.138, 0.156 and 320, respectively.

Figure 6.25: Dependence of lifetime enhancement on frequency for various duty cycles.

The inset shows the relationship between parameter K_1 and the duty cycle.

6.4.3 Model validation

Figure 6.26: Comparison between the measurement and model calculation. (a) Gate voltage dependence of DNBTI lifetime for difference frequencies/duty cycles; and (b) DNBTI lifetime and lifetime enhancement as function of operating temperature.

Figure 6.26 demonstrates the validation of the proposed model by showing the excellent agreement between the experimental and calculated DNBTI lifetime for different gate voltages/frequencies/duty cycles (Fig. 6.26a) and different operating temperatures (Fig. 6.26b). The same set of extracted parameter γ , α and K_2 is used to fit all the data in Fig. 6.25. Reasonably good agreement between the model and measurement data has been achieved for duty cycles ranging from 10 to 90 %, frequency ranging from DC to 500kHz, and different operating temperatures, showing the robustness of the model. In addition, both higher frequency and smaller duty cycle improve the device lifetime but the latter has a larger impact on the lifetime enhancement. This is confirmed by the Fig. 6.27 that depicting the 10-year lifetime operation voltages as a function of frequency and duty cycle. This suggests that one can improve the CMOS inverter lifetime by reducing the duty cycle of the input pulses. As expected, the lifetime enhancement should be independent of the temperature as shown in Fig. 6.26b), because the parameters γ , α and K_2 of Eq. (6.8) are independent of temperature.

Figure 6.27: Plot of 10-year lifetime operation voltage V_{dd} as a function of (a) frequency and (b) duty cycle. V_{dd} is based the criteria set in section 6.2.

6.4.4 On and off time dependence

From duty cycle experiment, it is difficult to identify whether degradation depends on T_{on} or/and T_{off} . Fig. 6.28 quantitatively shows the effect of T_{on} and T_{off} on lifetime enhancement factor under $DNBTI_{uni}$. The experimental results indicate that the lifetime enhancement factor depends strongly on the values of on and off time. This also confirms from another aspect that a frequency dependency for the DNBTI phenomenon. As T_{on} increases, the improvement diminishes and degradation approaches static level. On the contrary, degradation is reduced for smaller T_{on} or T_{off} . It is interesting to note that when the T_{off} approaches 10^{-8} s, regardless of different T_{on} , the lifetime enhancement diminishes. We believe the existence of this characteristic time (10^{-8} s) is related to the diffusion process. This would suggest that the dissociated hydrogen species need at least 10^{-8} s to reach the Si/SiO₂ interface for an effective annealing.

Figure 6.28: Dependence of lifetime enhancement ratio on T_{on} and T_{off} for $DNBTI_{inv}$.

6.5 Comparison of DNBTI degradation for different waveforms

Figure 6.29 depicts the comparison time dependence ΔV_{th} under 1 KHz and 100 KHz for (a) unipolar and (b) bipolar waveform. For comparison, ΔV_{th} under the same stress condition (i.e. $V_g=-2.2$ at 125 °C) is also included. Consistent with inverter-like waveform, it is evidently that both dynamic stress modes suppress NBTI-induced ΔV_{th} and improvement is enhanced when frequency increases as compared to SNBTI. More importantly, the bipolar stress exhibits the lowest ΔV_{th} as compared to unipolar. This is attributed to higher positive gate voltage applied during T_{off} which enhances recovery.

Figure 6.29: Comparison of time dependence ΔV_{th} under 1 KHz and 100 KHz for (a) unipolar $DNBTI_{uni}$ and (b) bipolar $DNBTI_{bi}$.

Figure 6.30 shows the device lifetime plot for pMOSFET under SNBTI, $\text{DNBTI}_{\text{inv}}$, $\text{DNBTI}_{\text{uni}}$ and DNBTI_{bi} . DNBTI_{bi} can significantly improve the lifetime by several orders of magnitude. The results shed light for the IC designers to suppress NBTI-induced reliability limitation through waveform optimization. On the other hand, nMOSFET in an inverter circuit has been reported that suffer from HCI (Hot Carrier Injection) during the transient period of an inverter-alike dynamic stress [199]. Thus, we propose the poor performance in $\text{DNBTI}_{\text{inv}}$ as compared to that of unipolar and bipolar is due to the occurrence of HC degradation during the transient period.

Figure 6.30: Comparison of device lifetime of pMOSFET under SNBTI, $\text{DNBTI}_{\text{inv}}$, $\text{DNBTI}_{\text{uni}}$, and DNBTI_{bi} .

Indeed, HSPICE simulation of an inverter circuit in Fig. 6.31 reveals the sequence of voltages applied to the FET gates. It is apparent that standard static NBTI evaluation represents only a subset of the various voltage applied and the dotted region denotes the HCI-dominated region. There is an observable drain current flow through the channel during the transient period suggesting that energetic carrier can be generated as a result of high lateral field. Based on this analysis, if the drain field in $\text{DNBTI}_{\text{inv}}$ is reduced, one would expect more annealing and/or less transient-induced HCI take place. To examine the effect of drain field on $\text{DNBTI}_{\text{inv}}$ -induced ΔV_{th} , we varied the positive gate-to-drain voltage, V_{gd} and result is shown in Fig. 6.32. For comparison, the effect of positive gate bias for bipolar stressing is included as reference. It is obvious that when V_{gd} is reduced from 2.2 to 1 V in $\text{DNBTI}_{\text{inv}}$ mode, the HCI-induced ΔV_{th} diminishes. On the contrary, the ΔV_{th} is reduced as V_{g_top} of DNBTI_{bi} increases. This indicates that more annealing can take place with increasing V_{g_top} in DNBTI_{bi} .

Figure 6.31: Calculated (a) V_g and V_d voltages and (b) the V_d voltage in an inverter at $\text{DNBTI}_{\text{inv}}$ stress conditions. (c) The V_g - V_d configurations applied on the pMOSFET during transient period. Dotted region means degradation is contributed by hot carrier effect.

Figure 6.32: Dependence of ΔV_{th} on the positive gate bias $V_{g,top}$ [$DNBTI_{bi}$] and V_{gd} [$DNBTI_{inv}$].

The transient-HCI in $DNBTI_{inv}$ can be attributed to the following two reasons. Firstly, the positive oxide charge generated during NBTI stress would definitely increase the localized drain field; hence produce a positive feedback mechanism, which worsen HCI [200]. Secondly, as shown in Chapter Four that NBTI-induced defect structures would weaken the nearby structures, therefore, it is expected that this bond weakening effect would deteriorate the HCI effect in pMOSFET during $DNBTI_{inv}$ stress.

6.5.1 Discussion on the frequency dependence of DNBTI

It has been previously reported that time-to-breakdown for thin SiO₂ films under bipolar and unipolar pulsed bias was greater than under dc stress [197],[198],[201]-[205]. The increase was attributed to enhanced de-trapping of holes at higher frequencies [203],[204]. The amount of the increase in lifetime is dependent on the fraction of holes detrapped in a given time interval. The fraction of holes detrapped was a function of the distance from the interface at which the holes were trapped. Later studies showed that the difference between oxide lifetime under pulsed and dc bias conditions became less as the voltage and oxide thickness were reduced [203]-[205]. In fact, no increase in lifetime under bipolar-pulsed bias was observed for 6.0 nm and 6.5 nm thick SiO₂ film [203],[204]. This is contradicting to what we observed in previous figure, which shows the dynamic stress enhancement over static stress remains significant for DNBTI despite the facts that T_{ox} is merely 1.8 nm. This indicates that a different physical mechanism may be responsible for the lifetime increase from that assumed in earlier studies for TDDB stress in thicker oxide. Therefore, we propose that the frequency dependence of DNBTI results can be explained by the enhanced recovery of NBTI-induced defects during high frequency.

The observed frequency dependence and, in particular, the lower degradation rate for the highest frequency can be qualitatively explained in the framework of the microscopic degradation model described in previous section. The transport stage of the process would play an important role, as it has been already suggested in previous works [202],[206],[207]. If the species released at the anode are charged [202],[206],[207], in our case refer to OH⁺, a reversal of the stress polarity or removing of stress would change their sense of movement so that the arrival of the cathode interface would be delayed. In

this way, if the stress frequency is low enough (longer semi-period), these hydrogen species will travel a longer distance in the oxide during the stressing interval before the polarity is changed. In contrast, if the stress frequency is very high, they will need a large number of stress cycles to reach the cathode, where they should finally generate a permanent defect at the Si/SiO₂ interface. This microscopic model is consistent to the dispersive transport model [208]–[210] and is illustrated in Fig. 6.33.

Figure 6.33: Illustration of dispersive transport model on various frequencies.

As observed from Fig. 6.23(b), the exponent time factor is well below 0.25 and decrease with higher frequency. Therefore, according to dispersive transport model for hydrogen diffusion species, smaller m suggests that dissociated hydrogen species experience more dispersive transport and take longer time to diffuse away from Si/SiO₂ interface in DNBTI_{inv} than that in SNBTI as illustrated in Fig. 6.32. Therefore, there are higher chances for the dissociated hydrogen species to re-passivate the NBTI-induced defects in DNBTI_{inv} than that in SNBTI. Hence, for the highest frequencies the generation of the defects at the interfaces would be delayed, leading to a slower degradation process and higher lifetime.

6.6 Chapter summary

Negative bias temperature instability under dynamic operation of a pMOSFET has been investigated. It is evidently shown that some of the NBTI-induced defects are annihilated when the stress is removed. This annealing is further enhanced by applying a positive gate bias or gate-to-drain bias during the device OFF period. The re-passivation of NBTI-induced interface trap and positive oxide charge are corroborated to be responsible for the recovery of NBTI-induced threshold voltage shift. More importantly, a same linearity is identified for both NBTI-induced degradation and anneal-induced recovery. This has given strong evidence that the recovery is due to the reverse reaction of NBTI degradation which comprise of detrapping of hydrogen-originated positive oxide charge and interactions between hydrogen species and the silicon dangling bonds. The model anticipates that some of the released hydrogen from Si-H dissociation process remains in the gate dielectric as positive oxide charge and they could diffuse back to the interface and passivate the interface trap.

A simple yet accurate lifetime model has been proposed to predict the life span of pMOSFET under dynamic operating condition. The fitting parameters of the model can be obtained from the calibration of one-time DNBTI lifetime measurement for a small set of frequency/duty cycle matrix. Excellent agreement between the model and the experiment is demonstrated. The model describes the behaviors of the NBTI lifetime enhancement excellently, and it has been shown that both higher frequency and smaller duty cycle can improve the device lifetime but the latter has a larger impact on the lifetime enhancement. The application of the model to the lifetime estimation of circuits with multiple operation modes is also discussed. In addition, a new degradation mode, in which transient HCI effect, is discovered when pMOSFET is stressed under inverter-alike

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waveform. Furthermore, the lifetime dependency on frequency is discussed and related to microscopic dispersive transport model.

CHAPTER SEVEN

Hydrogen-originated hole trapping (NBTI) reaction in high-K gate dielectric

In this chapter, NBTI in various potential high-k films are investigated and compared. It is found that Group IVB metal oxide has higher NBTI immunity than that of Group IIIA/IIIB based high-k and pure SiO₂. Although NBTI immunity of Group IVB silicate-based high-k films decreases NBTI reaction energy by 0.21 eV and 0.41eV for Zr-silicate and Hf-silicate, respectively as compared to their respective pure metal oxides, they are still energetically unfavorable for NBTI with reaction energy higher than that of SiO₂ by 0.64 eV and 0.83eV for Zr-silicate and Hf-silicate, respectively. In addition, Group IIIA/IIIB based high-k is a poor candidate for replacement of SiO₂ as far as NBTI is concerned. Furthermore, nitrogen-worsen NBTI remains a disturbing issue in high-k oxynitride based alloy. Based on these studies, two methods are proposed to suppress NBTI in high-k gate dielectrics.

7.1 Introduction

High-k gate dielectrics are being implemented in Si CMOS technologies to alleviate the rapid gate current increases associated with aggressive gate oxide thickness scaling. Replacement of SiO₂ as a gate dielectric is most urgent for low power circuits where gate leakage related power consumption is a serious limitation. Recent years, significant attention has been focused to improve thermal stability, fixed charge, charge trapping, mobility degradation and dopant penetration in different high-k films [211]-[214]. For details of pros and cons of different high-k dielectric films, one can refer to Ref. 219. However, in addition to these integration issues, implementation of a high-k gate dielectric also requires demonstration of its superior, if not, equivalent reliability performance with SiO₂. Moreover, negative bias temperature instability (NBTI) has become one of the dominant reliability concerns in advanced CMOS technologies. However, NBTI in high-k gate dielectrics has not been extensively investigated in spite of its importance. In this work, based on the atomic model proposed in Chapter Four, we compare the NBTI immunity for various potential high-k gate dielectrics using first-principles calculation. It is shown that Group IVB metal oxide has better NBTI immunity than that of Group IIIA/IIIB and pure SiO₂. Two methods are then proposed to suppress NBTI in high-k gate dielectric films.

7.2 Theoretical calculation and model validation

In this study, we use density functional theory (DFT) to study the NBTI reaction occurs in various high-k gate dielectric films. Specifically, we use B3LYP gradient-corrected DFT as like previous chapters. However, unlike previous calculations; all of the atoms are described using the Los Alamos LANL2 effective core potentials (ECP) and a valence double- ζ basis set. This is because mixed Gaussian basis set with split-valence-type plus polarization basis set is no longer adequate to describe the transition metal atoms or ions. Previous studies have shown the validity of this basis set and method on Hf and Zr [215],[216]. After the geometry optimization calculation, a frequency analysis is used to confirm its true minima state. From Table 1, it can be confirmed that our relaxed high-k models give a good representation of the local structure for various bonding configurations by comparing the bond lengths and the estimated band gap extracted from frontier molecular orbital with previous reported values [129],[217]-[219].

Table 7.1: Comparison of bond length and band gap of this work with other published works. A good agreement of bond lengths and band gaps is obtained indicating the validity of our high-k model.

Film studied	Respective bond	Bond Length (Å)		Bang gap (eV)	
		This work	Refs	This work	Ref. [219]
SiO ₂	Si-O	1.66	1.63 [217]	8.2	8.9
Si ₃ N ₄	Si-N	1.77	1.76 [129]	6.7	5.3
HfO ₂	Hf-O	1.92	1.96 [217]	5.8	6.0
Al ₂ O ₃	Al-O	1.70	1.76 [218]	6.7	8.7
ZrO ₂	Zr-O	1.95	1.94 [217]	5.3	5.8
La ₂ O ₃	La-O	2.18	-	4.2	4.3
Y ₂ O ₃	Y-O	2.03	-	4.2	5.6

7.3 Results and discussion

It has now recognized that the involvement of holes and Si-H bonds play a key role in NBTI. Recent study on NBTI in high-k film using the H₂O and D₂O as oxidant revealed that the involvement of hydrogen related defects [220]. Therefore, we assume that NBTI in high-k remains a hydrogen-originated process and thus, study on hydrogen-originated hole trapping reaction would be of importance to examine the NBTI performance for various possible high-k candidates. According to the model, interaction of inversion holes with the Si-H bonds at the Si/high-k interface of a pMOSFET results in dissociation of Si-H bonds, giving rise to interface traps. The dissociated H species would diffuse away and some of them are trapped by O bridge to generate positively charge defects in high-k films. Therefore, we study and compare the NBTI reaction energy (E_{NBTI}) of various high-k gate dielectrics as shown in Fig. 7.1. With SiO₂ film as a reference a negative ΔE_{NBTI} means NBTI easier to happen whereas a positive ΔE_{NBTI} means a more difficult reaction. From Fig. 7.1, reaction (ii) is energetically favorable by 0.99eV, explaining the well-known nitrogen-worsen NBTI effect. Among the high-k dielectrics given in Fig. 7.1, only HfO₂ and ZrO₂ have a positive ΔE_{NBTI} ($\Delta E_{\text{NBTI}} = 1.24$ eV for HfO₂ and $\Delta E_{\text{NBTI}} = 0.85$ eV for ZrO₂) and thus a higher resistance against NBTI as compared to SiO₂. The other high-k dielectrics including Al₂O₃, La₂O₃ and Y₂O₃ have a negative ΔE_{NBTI} , suggesting that they have a poorer NBTI immunity. Therefore, it can be concluded that Group IVB metal oxides have a higher NBTI immunity than both Group IIIA/IIIB metal oxides and SiO₂.

In addition, it is worth mentioning that all structures suffer interface degradation as upon trapping of H⁺, the over-coordinated complexes weaken the interface by the elongation of respective bond lengths [result not shown here]. This is consistent with

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finding observed in Chapter Four and seem to be the one of the common features for hydrogen trapping. This weakening interface will continue to pose serious reliability problem to pMOSFETs. Most important, it is found that the bond angle of trapping center deviates from its equilibrium angle upon trapping of released hydrogen for all high-k films. This is coherent with study in Chapter Five that suggests that interface strain continues to play an essential role in NBTI.

	NBTI reactions for various high-k gate dielectrics	ΔE_{NBTI} (eV)
(i) SiO_2	$\begin{array}{c} \diagup \text{Si} \diagdown \\ \\ \text{O} \\ \\ \diagdown \text{Si} \diagup \end{array} + \begin{array}{c} \text{Si} \\ \\ \text{Si}-\text{H} \\ \\ \text{Si} \end{array} \xrightarrow{h^+} \begin{array}{c} \text{Si} \\ \\ \text{Si}^{\bullet} \\ \\ \text{Si} \end{array} + \begin{array}{c} \text{H}^+ \\ \\ \text{O} \\ \\ \diagdown \text{Si} \diagup \end{array}$	0.0
(ii) Si_3N_4	$\begin{array}{c} \diagup \text{Si} \diagdown \\ \\ \text{N} \\ \\ \diagdown \text{Si} \diagup \\ \\ \text{Si} \end{array} + \begin{array}{c} \text{Si} \\ \\ \text{Si}-\text{H} \\ \\ \text{Si} \end{array} \xrightarrow{h^+} \begin{array}{c} \text{Si} \\ \\ \text{Si}^{\bullet} \\ \\ \text{Si} \end{array} + \begin{array}{c} \text{H}^+ \\ \\ \text{N} \\ \\ \diagdown \text{Si} \diagup \\ \\ \text{Si} \end{array}$	-0.99
(iii) HfO_2	$\begin{array}{c} \diagup \text{Hf} \diagdown \\ \\ \text{O} \\ \\ \diagdown \text{Hf} \diagup \end{array} + \begin{array}{c} \text{Si} \\ \\ \text{Si}-\text{H} \\ \\ \text{Si} \end{array} \xrightarrow{h^+} \begin{array}{c} \text{Si} \\ \\ \text{Si}^{\bullet} \\ \\ \text{Si} \end{array} + \begin{array}{c} \text{H}^+ \\ \\ \text{O} \\ \\ \diagdown \text{Hf} \diagup \end{array}$	1.24
(iv) ZrO_2	$\begin{array}{c} \diagup \text{Zr} \diagdown \\ \\ \text{O} \\ \\ \diagdown \text{Zr} \diagup \end{array} + \begin{array}{c} \text{Si} \\ \\ \text{Si}-\text{H} \\ \\ \text{Si} \end{array} \xrightarrow{h^+} \begin{array}{c} \text{Si} \\ \\ \text{Si}^{\bullet} \\ \\ \text{Si} \end{array} + \begin{array}{c} \text{H}^+ \\ \\ \text{O} \\ \\ \diagdown \text{Zr} \diagup \end{array}$	0.85
(v) Al_2O_3	$\begin{array}{c} \diagup \text{Al} \diagdown \\ \\ \text{O} \\ \\ \diagdown \text{Al} \diagup \end{array} + \begin{array}{c} \text{Si} \\ \\ \text{Si}-\text{H} \\ \\ \text{Si} \end{array} \xrightarrow{h^+} \begin{array}{c} \text{Si} \\ \\ \text{Si}^{\bullet} \\ \\ \text{Si} \end{array} + \begin{array}{c} \text{H}^+ \\ \\ \text{O} \\ \\ \diagdown \text{Al} \diagup \end{array}$	-0.33
(vi) La_2O_3	$\begin{array}{c} \diagup \text{La} \diagdown \\ \\ \text{O} \\ \\ \diagdown \text{La} \diagup \end{array} + \begin{array}{c} \text{Si} \\ \\ \text{Si}-\text{H} \\ \\ \text{Si} \end{array} \xrightarrow{h^+} \begin{array}{c} \text{Si} \\ \\ \text{Si}^{\bullet} \\ \\ \text{Si} \end{array} + \begin{array}{c} \text{H}^+ \\ \\ \text{O} \\ \\ \diagdown \text{La} \diagup \end{array}$	-2.13
(vii) Y_2O_3	$\begin{array}{c} \diagup \text{Y} \diagdown \\ \\ \text{O} \\ \\ \diagdown \text{Y} \diagup \end{array} + \begin{array}{c} \text{Si} \\ \\ \text{Si}-\text{H} \\ \\ \text{Si} \end{array} \xrightarrow{h^+} \begin{array}{c} \text{Si} \\ \\ \text{Si}^{\bullet} \\ \\ \text{Si} \end{array} + \begin{array}{c} \text{H}^+ \\ \\ \text{O} \\ \\ \diagdown \text{Y} \diagup \end{array}$	-1.13

Figure 7.1: NBTI reaction energy for various potential high-k gate dielectrics. The NBTI reaction energies are obtained from first-principles calculations after performing geometry optimization on both reactants and products. With SiO_2 as a reference a negative and positive ΔE_{NBTI} means that NBTI is energetically favorable and unfavorable respectively, as compared to SiO_2 . The unit of ΔE_{NBTI} is eV.

In addition to the above-mentioned metal oxides, silicates based on Group IVB and Group IIIA/IIIB metals could be used as high-k gate dielectrics also. The reaction energies for these silicates have been calculated and are shown in Fig.7.2. As compared to pure SiO₂, the silicates based on Group IVB metals still have a better NBTI immunity while the silicates based on Group IIIA/IIIB metals still have a poorer NBTI immunity. This is consistent with the trend of the metal oxides observed in Fig. 7.1. However, a comparison between Figs. 7.1 and 7.2 reveals that the reaction energies of the Hf- and Zr-based silicates are lower than those of the pure Hf and Zr oxides by 0.41eV and 0.21eV, respectively.

NBTI reactions for various silicate based high-k gate dielectrics	ΔE_{NBTI} (eV)
(i) Hf-Silicate $\text{Hf-O-Si} + \text{Si-Si-H} \xrightarrow{h^+} \text{Si-Si} + \text{Hf-O-Si}^+$	0.83
(ii) Zr-Silicate $\text{Zr-O-Si} + \text{Si-Si-H} \xrightarrow{h^+} \text{Si-Si} + \text{Zr-O-Si}^+$	0.64
(iii) Al-Silicate $\text{Al-O-Si} + \text{Si-Si-H} \xrightarrow{h^+} \text{Si-Si} + \text{Al-O-Si}^+$	-0.20
(iv) La-Silicate $\text{La-O-Si} + \text{Si-Si-H} \xrightarrow{h^+} \text{Si-Si} + \text{La-O-Si}^+$	-0.65
(v) Y-Silicate $\text{Y-O-Si} + \text{Si-Si-H} \xrightarrow{h^+} \text{Si-Si} + \text{Y-O-Si}^+$	-0.28

Figure 7.2: NBTI reaction energy for various silicate based high-k gate dielectrics with SiO₂ as a reference. Group IVB is energetically unfavorable for NBTI as compared to Group IIIA/IIIB and SiO₂.

The above results suggest that the silicates based on Group IVB metals have a poorer NBTI immunity than the corresponding metal oxides. In contrast, the silicates based on Group IIIA/IIIB metals have higher reaction energy and thus a better NBTI immunity than the corresponding pure metal oxides. These results are self-explanatory, and they can be explained as follows. The NBTI immunity of SiO_2 is poorer than that of Hf and Zr oxides but better than that of Al, La and Y oxides. Therefore, in the silicates based on Hf or Zr, one Hf or Zr atom is replaced by one Si atom and thus the reaction energy should be lower as compared to the corresponding metal oxide. Similarly, one Al or La or Y atom is substituted by one Si atom in the silicate based on Group IIIA/IIIB metals; as a result the reaction energy should be higher as compared to the corresponding metal oxide.

On the other hand, aluminate- and oxynitride-based high-k alloys have shown an improved thermal stability, and thus it is necessary to examine their NBTI immunity. As shown in Fig. 3, adding Al_2O_3 into the HfO_2 and ZrO_2 inevitably lowers the E_{NBTI} by 0.64 and 0.42eV in relative to the corresponding pure metal oxides, respectively. However, this tradeoff for the improved stability is still acceptable, because the reaction energies of Zr-aluminate and Hf-aluminate are still higher than that of pure SiO_2 by 0.43eV and 0.60eV, respectively. As Al_2O_3 has lower reaction energy than HfO_2 and ZrO_2 , the reduction of reaction energy of the aluminate-based alloys can be explained by the substitution of one Hf or Zr atom by one Al atom. On the other hand, negative ΔE_{NBTI} values, i.e., -0.32 eV for Hf-oxynitride, -0.73eV for Zr-oxynitride and -0.81 eV for , Al-oxynitride are observed. This suggests that adding oxynitride into HfO_2 , ZrO_2 and Al_2O_3 significantly lower the NBTI immunity to the extent that is even poorer than SiO_2 . This result is disturbing because oxynitride is added with the aim of increasing the thermal

stability of the high-k dielectrics. Obviously, the nitrogen-enhanced NBTI effect remains as a severe issue in high-k oxynitride films. The results are consistent with previous experimental work [221] which showed that nitrogen in HfO₂ exacerbates NBTI degradation.

NBTI reactions for various aluminate based high-k gate dielectrics	ΔE_{NBTI}
(i) Hf-Aluminate $\begin{array}{c} \diagup \text{Hf-O-Al} \diagdown \\ \diagup \quad \quad \diagdown \end{array} + \begin{array}{c} \text{Si} \\ \diagup \quad \diagdown \\ \text{Si-Si-H} \\ \diagdown \quad \diagup \\ \text{Si} \end{array} \xrightarrow{h^+} \begin{array}{c} \text{Si} \\ \diagup \quad \diagdown \\ \text{Si-Si} \cdot \\ \diagdown \quad \diagup \\ \text{Si} \end{array} + \begin{array}{c} \text{H}^+ \\ \diagup \quad \diagdown \\ \text{Hf-O-Al} \\ \diagdown \quad \diagup \end{array}$	0.60
(ii) Zr-Aluminate $\begin{array}{c} \diagup \text{Zr-O-Al} \diagdown \\ \diagup \quad \quad \diagdown \end{array} + \begin{array}{c} \text{Si} \\ \diagup \quad \diagdown \\ \text{Si-Si-H} \\ \diagdown \quad \diagup \\ \text{Si} \end{array} \xrightarrow{h^+} \begin{array}{c} \text{Si} \\ \diagup \quad \diagdown \\ \text{Si-Si} \cdot \\ \diagdown \quad \diagup \\ \text{Si} \end{array} + \begin{array}{c} \text{H}^+ \\ \diagup \quad \diagdown \\ \text{Zr-O-Al} \\ \diagdown \quad \diagup \end{array}$	0.43
NBTI reactions for various oxynitride based high-k gate dielectrics	ΔE_{NBTI}
(i) Hf-Oxynitride $\begin{array}{c} \diagup \text{Hf-N-Hf} \diagdown \\ \diagup \quad \quad \diagdown \\ \text{Hf} \end{array} + \begin{array}{c} \text{Si} \\ \diagup \quad \diagdown \\ \text{Si-Si-H} \\ \diagdown \quad \diagup \\ \text{Si} \end{array} \xrightarrow{h^+} \begin{array}{c} \text{Si} \\ \diagup \quad \diagdown \\ \text{Si-Si} \cdot \\ \diagdown \quad \diagup \\ \text{Si} \end{array} + \begin{array}{c} \text{H}^+ \\ \diagup \quad \diagdown \\ \text{Hf-N-Hf} \\ \diagdown \quad \diagup \\ \text{Hf} \end{array}$	-0.32
(ii) Zr-Oxynitride $\begin{array}{c} \diagup \text{Zr-N-Zr} \diagdown \\ \diagup \quad \quad \diagdown \\ \text{Zr} \end{array} + \begin{array}{c} \text{Si} \\ \diagup \quad \diagdown \\ \text{Si-Si-H} \\ \diagdown \quad \diagup \\ \text{Si} \end{array} \xrightarrow{h^+} \begin{array}{c} \text{Si} \\ \diagup \quad \diagdown \\ \text{Si-Si} \cdot \\ \diagdown \quad \diagup \\ \text{Si} \end{array} + \begin{array}{c} \text{H}^+ \\ \diagup \quad \diagdown \\ \text{Zr-N-Zr} \\ \diagdown \quad \diagup \\ \text{Zr} \end{array}$	-0.73
(iii) Al-Oxynitride $\begin{array}{c} \diagup \text{Al-N-Al} \diagdown \\ \diagup \quad \quad \diagdown \\ \text{Al} \end{array} + \begin{array}{c} \text{Si} \\ \diagup \quad \diagdown \\ \text{Si-Si-H} \\ \diagdown \quad \diagup \\ \text{Si} \end{array} \xrightarrow{h^+} \begin{array}{c} \text{Si} \\ \diagup \quad \diagdown \\ \text{Si-Si} \cdot \\ \diagdown \quad \diagup \\ \text{Si} \end{array} + \begin{array}{c} \text{H}^+ \\ \diagup \quad \diagdown \\ \text{Al-N-Al} \\ \diagdown \quad \diagup \\ \text{Al} \end{array}$	-0.81

Figure 7.3: NBTI reaction energy for various aluminate and oxynitride based high-k gate dielectrics with SiO₂ as a reference. Obviously, nitrogen remains a disturbing problem in high-k gate dielectrics.

Chapter 7: Hydrogen-originated hole trapping (NBTI) reaction in high-K gate dielectric

Based on the results, we propose two methods to suppress NBTI in high-k gate dielectric and at the same time maintaining the improvement in terms of thermal stability and lowering the fixed-charge induced mobility degradation. First method is to employ laminated high-k method [1] with HfO_2 being deposited prior to Al_2O_3 deposition since HfO_2 has higher NBTI immunity than that of Al_2O_3 . Second method is employ Hf-rich interfacial layer to increase the coordination number of O at the interface [222] to minimize the NBTI reaction sites. As cited earlier, O lone pair is the reaction site responsible for the trapping of released hydrogen, thus, increase of O coordination number by Hf-rich film can minimize the reaction site.

7.4 Chapter summary

We have studied the NBTI resistance for various potential high-k gate dielectric layers. From the calculation of NBTI reaction energy, Group IVB metal oxides are found to have better NBTI immunity as compared to Group IIIA/IIIB and SiO_2 . Furthermore, Group IVB silicate is found to have relatively high NBTI immunity. However, nitrogen remains a disturbing reliability issue in all the above-mentioned dielectrics. In this study, we have proposed two methods to suppress NBTI based on HfO_2 .

CHAPTER EIGHT

Conclusions and Recommendations

8.1 Conclusions

This chapter briefly summarizes the work presented in this thesis. This thesis has addressed one of the key reliability challenges, namely negative bias temperature instability (NBTI), which is associated with the electrical characterization and atomic modeling of the ultra-thin gate dielectric in advanced MOSFETs. These studies enhance the understanding of NBTI reliability for advanced technologies. Finally, the directions for future work are pointed out.

8.1.1 Nitrogen-worsen NBTI effect

The influence of interfacial nitrogen concentration on the time, oxide field and temperature dependence of the NBTI-induced threshold voltage shift has been quantitatively studied. Although nitrogen has negligible effect on time exponent and oxide field accelerator, it has strong impact on the temperature dependence of NBTI. Furthermore, both positive oxide charge and interface trap are confirmed to be the primary defects responsible for threshold voltage shift and device parameter degradation in both pure SiO_2 and nitrided oxides and both positive oxide charge trapping and interface trap generation increase proportionally with interfacial nitrogen concentration. It

has been further concluded that enhanced generation of interface trap and positive oxide charge is attributed to reduce thermal activation energies with increasing interfacial nitrogen concentration. In addition, based on the nitrogen profile experiment, it is concluded that nitrogen at the interface plays a dominating role in the enhancement effect. It is found that hydrogen-related defect e.g. Si-H is the origin for NBTI in pure SiO₂ and nitrided oxide. More importantly, nitrogen and hydrogen must present for the enhancement of threshold voltage shift whereas vacancy defect plays a trivial role in NBTI.

The experimental finding can be explained by atomic modeling of NBTI. In this model, NBTI for both pure SiO₂ and nitrided oxide can be described by hydrogen-originated hole trapping reaction. It has been demonstrated from first-principles total-energy calculation that nitrogen can be an efficient trapping center for released hydrogen ion as compared to oxygen. Furthermore, the NBTI degradation dependence of N_{int} at two distinct regions, namely, $N_{\text{int}} > 8$ atomic % and $N_{\text{int}} < 8$ atomic %, is due to the effect of N atoms surrounding a Si atom. With this N neighboring effect, the reduction of reaction energy for the NBTI reaction with increasing the N_{int} is faster for two-N atom structure (N₂-Si-O₂) than one-N atom structure (N-Si-O₃). This N neighboring effect on the enhancement of the NBTI degradation is detrimental to future generations of MOS devices that require higher N_{int} for the gate oxide.

On the other hand, we have experimentally demonstrated that the transition layer near the Si/SiO₂ interface might have strong impact on the NBTI degradation of ultra-thin gate oxide. The experimental proposition has been confirmed by the theoretical study using first-principles calculation. The calculations have shown that the bond strength of NBTI precursor, that is Si-H, is strongly weakened by the interfacial strain. Furthermore,

the reaction energy of hydrogen-originated hole trapping reaction is lowered by the interfacial strain. Although both compressive stress and tensile stress enhance NBTI, the former seems to have larger influence than the later one. This is disturbing, as the compressive stress is always present at Si/SiO₂ interface. Conversely, the effect of stoichiometry oxide on NBTI is less problematic. It is observed that Si-H bond strength is weaker when reside at sub-stoichiometric oxide than at stoichiometric oxide and they are slightly weaker at Si/SiO_xN_y interface than at Si/SiO₂ interface. Unlike interfacial strain, the reaction energy of hydrogen-originated hole trapping reaction is not affected by stoichiometric oxide. In short, controlling of the strain layer property within 1nm thick is extremely important for future ultra-thin gate oxides with high reliability in sub-65 nm ULSI technology. Therefore, relaxation of the strained-layer is a requisite issue to improve reliability and realize the aggressive scaling.

Nitrogen-worsen NBTI effect cannot be simply explained by a single or double factor. As demonstrated, nitrogen at Si/SiO_xN_y has multiple negative effects: (1) it creates more NBTI precursors (that is more N and Si-H bond); (2) it lowers the NBTI reaction energy; (3) it slightly weaken the Si-H bond strength and finally, (4) it increases the susceptibility against strain-enhanced NBTI effect. The lowering of NBTI reaction energy can be understood from the fact the nitrogen is less electronegativity than oxygen and larger negative charge at nitrogen provides a more effective Coulombic attraction center for trapping of positive charge like H⁺. After NBTI, the localized bridging structure is weakened and gap state is generated within the oxide band gap and the oxide band gap is lowered. This pose a serious threat to another reliability issues such hot carrier issue.

8.1.2 Suppression of NBTI

Based on the current understanding of NBTI, reducing the nitrogen content at the interface is inevitable to prevent deterioration of NBTI degradation. However, nitrogen is required to prevent boron penetration. Thus, nitrogen profile engineering e.g. plasma nitridation is essential to suppress NBTI. In this regard, plasma nitridation can displace the peak nitrogen profile away from the interface, hence, reducing the nitrogen content at the interface. This can alleviate the nitrogen enhancement effect as well as boron penetration problem. However, plasma nitridation shall face greater challenge to keep the peak nitrogen near oxide surface due to aggressive oxide scaling and increasingly thermal budget in future technologies. Thus, it should only be a short-term solution to suppress NBTI. In addition to plasma nitridation, relaxation of the strained-layer is a requisite issue to improve the NBTI reliability. To do this, steam oxide like in-situ steam generation (ISSG) can be employed to obtain better interfacial quality. Therefore, combining ISSG and plasma nitridation, we should obtain a greater improvement in term of higher NBTI immunity. Nevertheless, a careful optimization of post nitridation annealing is also essential to suppress NBTI.

Another way to suppress NBTI from a long-term point of view is to address the minimization of NBTI precursor. In this regard, deuterium and fluorine annealing would be the superior candidate than hydrogen to terminate the Si dangling bond in terms of bond energy. The stronger Si-D and Si-F would further reduce NBTI.

8.1.3 Dynamic NBTI in PMOS Transistor

Although NBTI degradation can be quite a serious issue in static stress mode, it has been evidently shown that some of the NBTI-induced defects are annihilated when the stress is removed. This annealing can be further enhanced by applying a positive gate bias or gate-to-drain bias during the device OFF period. The re-passivation of NBTI-induced interface trap and positive oxide charge are corroborated to be responsible for the recovery of NBTI-induced threshold voltage shift. More importantly, a same linearity is identified for both NBTI-induced degradation and anneal-induced recovery. This has given a strong evident that the recovery is due to the reverse reaction of NBTI degradation which comprise of detrapping of hydrogen-originated positive oxide charge and interactions between hydrogen species and the silicon dangling bonds. The recovery model anticipates that some of the released hydrogen from Si-H dissociation process remains in the gate dielectric as positive oxide charge and they could diffuse back to the interface and passivate the interface trap.

A simple yet accurate lifetime model has been proposed to predict the life span of pMOSFET under dynamic operating condition. The fitting parameters of the model can be obtained from the calibration of one-time dynamic NBTI (DNBTI) lifetime measurement for a small set of frequency/duty cycle matrix. Excellent agreement between the model and the experiment is obtained. The model describes the behaviors of the NBTI lifetime enhancement excellently, and it has been shown that both higher frequency and smaller duty cycle can improve the device lifetime with the latter having a larger impact on the lifetime enhancement. The application of the model to the lifetime estimation of circuits with multiple operation modes is also discussed. In addition, a new degradation mode, transient HCI effect, is discovered when pMOSFET is stressed under inverter-alike

waveform. Thus, circuit design needs to take the NBTI degradation into account in addition to HC effects in optimizing the trade off between circuit performance requirements and reliability targets. Finally, the lifetime dependency on frequency is discussed and related to microscopic dispersive transport model.

8.1.4 Hydrogen-originated hole trapping (NBTI) reaction in high-K gate dielectric

The NBTI immunity for various potential high-k gate dielectric layers has been studied theoretically. From the calculation of NBTI reaction energy, Group IVB metal oxides are found to have better NBTI immunity compared to Group IIIA/IIIB and SiO₂. Furthermore, Group IVB silicate is found to have relatively high NBTI immunity. However, nitrogen remains a disturbing reliability issue in all the above-mentioned dielectrics. In this study, two methods to suppress NBTI based on HfO₂ are proposed.

8.2 Recommendations

8.2.1 Physical mechanism of Si-H dissociation by cold hole

Based on the experimental observation, it has been accepted that hole from inversion layer responsible to break the Si-H bond. Fundamentally it remains uncertain that how the cold holes accelerated by operating voltage as low as 2.2 V in this work can break the Si-H bond and generate the interface traps. This is a big unsolved issue and probably more complicated processes such as the Auger mechanism may be involved [223]-[227] or weakening of Si-H bond to the interfacial strain. It is almost undeniable that interfacial strain is one of the important factors that responsible for NBTI degradation in ultra-thin gate dielectric and it has been theoretically shown in Chapter Five that the Si-H bond strength can be severely weaken by interfacial strain. More experimental works are needed to understand how the cold holes from the inversion layer dissociate the Si-H bond. Is it related to Auger mechanism-induced dissociation or weakening of Si-H bond due to the increasing interfacial strain as a result of aggressive gate dielectric thickness scaling?

8.2.2 Identification of diffusion species

From Chapters Four and Six, it has been generalized that the diffusion species should be hydrogen-related structures, e.g. H^0 , H^+ , H_2 or even H_3O^+ . Through various experimental results, it has been suggested that H^+ is most likely the diffusion species, a clear identification of the diffusion species is not yet achieved. This is crucial as it can help to determine a more accurate electrochemical reaction and rate-limiting reaction.

8.2.3 Impact of NBTI effect on analog circuit

Analog circuits using matched pairs (differential pairs, current mirrors), are designed to be relatively insensitive to transistor matched threshold voltage and shifts of the pair, but are much more sensitive to increases in threshold voltage and mismatches between the pair due to aging. Thus, NBTI may cause mismatch shifts due to random variations in the number and spatial distribution of the charges formed during the NBTI aging. This poses serious reliability issue for analog circuit. However, such study on analog circuit is still lacking. Furthermore, the impact of nitrogen-worsen NBTI on analog circuit is also of critical issue.

8.2.4 Dynamic NBTI Lifetime model for multiple operation modes circuit

The simple lifetime model proposal in Chapter Six consider the average impact of various operation modes, this is not exactly true as degradation mechanism for each operation mode might be different. For a complete work for circuit simulation, a novel DNBTI lifetime model to accommodate different operation modes is essential since circuits are used to operate under various operation modes. For greater accuracy, the interaction of NBTI-Hot carrier effect must be taken into account.

8.2.5 NBTI in high-K gate dielectric

According to ITRS roadmap, it might be necessary to have high-k gate dielectric for production as soon as year 2005 in order to meet the leakage current specification for some low power IC applications. Clearly, no material can be used in production until reliability issue such as NBTI is established. Therefore, there is a pressing need to study

Chapter 8: Conclusions and Recommendations

NBTI of promising high-k dielectrics such as HfO_2 . This work is still nascent. While it appears that HfO_2 is sufficiently immune to hot-carrier degradation [228], NBTI issue in pMOSFET has not been addressed. Theoretical work based on the assumption that NBTI in high-k can be well described by hydrogen-originated hole trapping reaction has been carried to understand the NBTI immunity among the potential high-k gate dielectric. Experimental works are required to justify the speculation.

List of publications

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7. **S. S. Tan**, T. P. Chen and C. H. Ang, ""Influences of nitridation on tunneling barrier change and charge trapping caused by electrical stress," *J. Appl. Phys.* vol. 93 No. 5, pg 3114-3116, (2003).
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9. J. M. Soon, K. P. Loh, **S. S. Tan**, T. P. Chen, W. Y. Teo and L. Chan, "Study of negative bias temperature instability induced defects using first principles approach," *Appl. Phys. Lett.* vol. 83 No. 15, pg.3063-3065, (2003).
10. **S. S. Tan**, T. P. Chen, C. H. Ang and L. Chan, "Mechanism of nitrogen-enhanced negative bias temperature instability in pMOSFET," (**invited paper**) *Mircoelec. Relia.*, in press.
11. **S. S. Tan**, T. P. Chen, J. M. Soon, K. P. Loh, C. H. Ang and L. Chan, " On the effects of local topology on Si-H bond energy and vacancy formation and their role in negative bias temperature instability," to be submitted.
12. **S. S. Tan**, T. P. Chen, C. H. Ang and L. Chan, "Atomic modeling of nitrogen neighboring effect on negative bias temperature instability of pMOSFETs," *IEEE Elec. Dev. Lett.* 25, 504, 2004.
13. **S. S. Tan**, T. P. Chen, C. H. Ang and L. Chan, "Impact of interfacial strain on negative bias temperature instability," to be submitted.
14. **S. S. Tan**, T. P. Chen, C. H. Ang and L. Chan, "Mechanism of annealing effect in dynamic negative bias temperature instability," to be submitted.

List of publications

15. **S. S. Tan**, T. P. Chen, C. H. Ang and L. Chan, "Comparison of NBTI immunity among the various potential high-k gate dielectric films," to be submitted.

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Appendix A

QBasic Program for Static NBTI measurement:

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100 !*****
110 !*
120 !* NBTI Static Stress/Masurement Test
130 !*
140 !* Edit History:
162 !* Created by Shyue Seng Tan on 18 Aug 2001
170 !*****
180 COM @Hp415x,@Form_off,INTEGER Hpib_sc,Swm
190 COM /File_name1/ Idlin_file$[12],Idsat_file$[12],Str_file$[12]
200 COM /File_name3/ Idlin_data$[100],Gmmax_data$[100],Vtext_data$[100]
210 COM /File_name4/ Idsat_data$[100]
220 COM /Meas_info1/ INTEGER Meas_points,Present,REAL Meas_str_time(1:100)
230 COM /Meas_info4/ INTEGER Gate_str,Source_str,Drain_str,Bulk_str
240 COM /Meas_info5/ REAL Vdstr,Vgstr,Vdd,Vbb,Gate_length,Gate_width
250 COM /Meas_data1/ REAL Idlin_init,Idlin_shift(1:100)
260 COM /Meas_data2/ REAL Gmmax_init,Gmmax_shift(1:100),Vtext_init,Vtext_shift(1:100)
270 COM /Meas_data3/ REAL Idsat_init,Idsat_shift(1:100)
280 COM /Smu/ Vg$[4],Vs$[4],Vd$[4],Vb$[4]
290 !
300 ! ----- HP-IB Setup -----
310 INTEGER Hpib_addr,Swm_sc,Swm_addr
320 !
330 Hpib_sc=8      ! HP 415X HP-IB Select Code
340 Hpib_addr=0    ! HP 415X HP-IB Address
350 !
360 ASSIGN @Hp415x TO Hpib_sc*100+Hpib_addr
370 ASSIGN @Form_off TO Hpib_sc*100+Hpib_addr;FORMAT OFF
380 !
390 ! ----- Input Parameters -----
400 Vs$="SMU4"      !Vs$="SMU3"   Characterization Lab
410 Vg$="SMU1"      !Vg$="SMU2"
420 Vd$="SMU2"      !Vd$="SMU1"
430 Vb$="SMU3"      !Vb$="SMU4"
440 Meas_points=17   ! Number of times to repeat measurements
450 REDIM Meas_str_time(1:Meas_points)
460 REDIM Idlin_shift(1:Meas_points),Gmmax_shift(1:Meas_points),Vtext_shift(1:Meas_points)
470 REDIM Idsat_shift(1:Meas_points)
480 !
490 ! ----- Stress Condition for NBTI -----
500 Vdstr=0          ! Drain stress voltage
510 Vgstr=-2.2       ! Gate stress voltage
520 ! ----- Measurement Condition -----
530 Vdd=-1.0         ! Drain nominal voltage
540 Vbb=0            ! Bulk nominal voltage
545 Condition$="S18120002 W#16 18A"
546 Condition1$="Vg=-2.2V Vg=+0V"
547 Condition2$="T=125C 100/1um"
548 Condition3$="Vdd=-1V Vgb=-0.3V"
550 !

```

Appendix

```

560 ! ----- Device geometries -----
570 Gate_length=1.2E-7 ! Gate length
580 Gate_width=1.0E-5 ! Gate width
590 !
600 ! ----- Definition of measurement and stress setup files -----
610 !
620 Str_file$="NBTI.STR" ! DC stress setup file
630 Idlin_file$="IDLIN.MES" ! Idlin/Gmmax/Vtext/Vtci measurement setup file
640 Idsat_file$="IDSAT.MES" ! Idsat measurement setup file
650 !
660 ! ----- File name to save ASCII data -----
670 Idlin_data$="IDLIN" ! Idlin shift data file name
680 Gmmax_data$="GM" ! Gmmax shift data file name
690 Vtext_data$="VTH" ! Vtext shift data file name
700 Idsat_data$="IDSAT" ! Idsat shift data file name
710 !
720 ! ----- Stress duration setup -----
730 Str_time: ! ! Stress duration data
740 DATA 1, 2, 5
750 DATA 10, 20, 50
760 DATA 100, 200, 500
770 DATA 1000, 2000, 5000
772 DATA 10000, 20000, 30000
774 DATA 40000, 50000, 60000
780 RESTORE Str_time
790 READ Meas_str_time(*)
800 !
810 !!!!!!!!!!!!! Main !!!!!!!!!!!!!
820 !
830 CALL Initial_setting ! Initial setting
840 CALL Init_hp415x ! Initialize HP 415X
850 CREATE Idlin_data$,100
860 CREATE Gmmax_data$,100
870 CREATE Vtext_data$,100
880 CREATE Idsat_data$,100
883 CREATE "Testcon",10
884 ASSIGN @File TO "Testcon";FORMAT ON
885 OUTPUT @File;Condition$
886 OUTPUT @File;Condition1$
887 OUTPUT @File;Condition2$
888 OUTPUT @File;Condition3$
889 ASSIGN @File TO *

890 ! --- Initial Characterization ---
900 Present=0
910 CALL Idsat_meas ! Initial Idsat characterization
920 CALL Idlin_meas ! Initial Idlin characterization
930 !CALL Record_idsdata ! Record Idsat_shift data
940 !CALL Record_iddata ! Record Idlin_shift data
950 !CALL Record_gmdata ! Record Gmmax_shift data
960 !CALL Record_vtdata ! Record Vtext_shift data

970 !
980 ! ----- Stress/measurement cycle Characterization -----
990 FOR Present=1 TO Meas_points ! Start stress/measurement cycles
1000 CALL Stress ! Increment stress time and force stress
1010 CALL Idsat_meas ! Interim measurement

```

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1020 CALL Idlin_meas          ! Interim measurement
1030 NEXT Present
1032 CALL Record_idsdata     ! Record Idsat_shift data
1040 CALL Record_iddata      ! Record Idlin_shift data
1050 CALL Record_gmdata      ! Record Gmmax_shift data
1060 CALL Record_vtedata     ! Record Vtext_shift data
1080 DISP "NBTI Test is Completed!!"
1090 !
1100 END
1110 !!!!!!!!!!!!! Sub !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
1120 Initial_setting:SUB Initial_setting
1130 COM @Hp415x,@Form_off,INTEGER Hpib_sc,Swm
1140 COM /File_name1/ Idlin_file$[12],Idsat_file$[12],Str_file$[12]
1150 COM /File_name3/ Idlin_data$[100],Gmmax_data$[100],Vtext_data$[100]
1160 COM /File_name4/ Idsat_data$[100]
1170 COM /Meas_info1/ INTEGER Meas_points,Present,REAL Meas_str_time(*)
1180 COM /Meas_info4/ INTEGER Gate_str,Source_str,Drain_str,Bulk_str
1190 COM /Meas_info5/ REAL Vdstr,Vgstr,Vdd,Vbb,Gate_length,Gate_width
1200 COM /Meas_data1/ REAL Idlin_init,Idlin_shift(*)
1210 COM /Meas_data2/ REAL Gmmax_init,Gmmax_shift(*),Vtext_init,Vtext_shift(*)
1220 COM /Meas_data3/ REAL Idsat_init,Idsat_shift(*)
1230 !
1240 COM /Smu/ Vg$,Vs$,Vd$,Vb$
1250 SUBEND
1260 Init_hp415x:SUB Init_hp415x
1270 COM @Hp415x,@Form_off,INTEGER Hpib_sc,Swm
1280 COM /File_name1/ Idlin_file$[12],Idsat_file$[12],Str_file$[12]
1290 COM /File_name3/ Idlin_data$[100],Gmmax_data$[100],Vtext_data$[100]
1300 COM /File_name4/ Idsat_data$[100]
1310 COM /Meas_info1/ INTEGER Meas_points,Present,REAL Meas_str_time(*)
1320 COM /Meas_data1/ REAL Idlin_init,Idlin_shift(*)
1330 COM /Meas_data2/ REAL Gmmax_init,Gmmax_shift(*),Vtext_init,Vtext_shift(*)
1340 COM /Meas_data3/ REAL Idsat_init,Idsat_shift(*)
1350 COM /Meas_info4/ INTEGER Gate_str,Source_str,Drain_str,Bulk_str
1360 COM /Meas_info5/ REAL Vdstr,Vgstr,Vdd,Vbb,Gate_length,Gate_width
1370 COM /Smu/ Vg$[4],Vs$[4],Vd$[4],Vb$[4]
1380 !
1390 CLEAR SCREEN
1400 CLEAR @Hp415x
1410 OUTPUT @Hp415x;"*RST"          ! Device reset
1420 OUTPUT @Hp415x;"*CLS"          ! Clear status data
1430 OUTPUT @Hp415x;".STAT:PRES"    ! Preset event enable mask register
1440 OUTPUT @Hp415x;".DISP:WIND:STAT OFF" ! Screen update off
1450 OUTPUT @Hp415x;".CAL:AUTO OFF"  ! Auto calibration off
1460 OUTPUT @Hp415x;"*ESE 60;*SRE 32;*OPC?" ! Event status/service request enable register
setup
1470 ENTER @Hp415x;A
1480 OUTPUT @Hp415x;".DISP:WIND:ALL BST" ! Display IBASIC status screen
1485 OUTPUT @Hp415x;".PAGE:SCON:STAN ON" ! Standby ON
1490 !
1500 ! Load initial/interim characterization setup file into internal memory
1510 !
1520 OUTPUT @Hp415x;".MMEM:LOAD:STAT 0,"&Idlin_file$&","'DISK'"
1530 OUTPUT @Hp415x;".PAGE:MEAS:SWE:VAR1:STOP "&VAL$(Vdd)
1540 OUTPUT @Hp415x;".PAGE:MEAS:SWE:CONS:"&Vb$&" "&VAL$(Vbb)
1541 !!!!!!! KEY IN Transistor Width and Length !!!!!!!
1542 OUTPUT @Hp415x;".PAGE:CHAN:UFUN:DEF 'W','um','10'"

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1544 OUTPUT @Hp415x;":PAGE:CHAN:UFUN:DEF 'L','um','0.12'"
1546 OUTPUT @Hp415x;":PAGE:DISP:ANAL:MARK:POS 'ID', '-0.1E-6*W/L'"
1550 OUTPUT @Hp415x;":MMEM:STOR:STAT 0,'MEM1.MES','MEMORY'"
1560 OUTPUT @Hp415x;":MMEM:DEL ""&Idlin_file$&""', 'DISK', "
1570 OUTPUT @Hp415x;":MMEM:STOR:STAT 0, ""&Idlin_file$&""', 'DISK'"
1580 OUTPUT @Hp415x;":MMEM:LOAD:STAT 0, ""&Idsat_file$&""', 'DISK'"
1590 OUTPUT @Hp415x;":PAGE:MEAS:SWE:VAR1:STOP "&VAL$(Vdd)
1600 OUTPUT @Hp415x;":PAGE:MEAS:SWE:CONS:"&Vb$&" "&VAL$(Vbb)
1610 OUTPUT @Hp415x;":MMEM:STOR:STAT 0,'MEM3.MES','MEMORY'"
1620 OUTPUT @Hp415x;":MMEM:DEL ""&Idsat_file$&""', 'DISK', "
1630 OUTPUT @Hp415x;":MMEM:STOR:STAT 0, ""&Idsat_file$&""', 'DISK'"
1640 !
1650 ! Load stress setup file to HP 4155A/4156A
1660 !
1670 OUTPUT @Hp415x;":MMEM:LOAD:STAT 0, ""&Str_file$&""', 'DISK'"
1680 OUTPUT @Hp415x;":PAGE:STR:SET:CONS:"&Vd$&" "&Vdstr
1690 OUTPUT @Hp415x;":PAGE:STR:SET:CONS:"&Vg$&" "&Vgstr
1700 OUTPUT @Hp415x;":PAGE:STR:SET:CONS:"&Vb$&" "&Vbb
1710 OUTPUT @Hp415x;":MMEM:DEL ""&Str_file$&""', 'DISK'"
1720 OUTPUT @Hp415x;":MMEM:STOR:STAT 0, ""&Str_file$&""', 'DISK'"
1730 !
1740 SUBEND
1750 !
1760 Idlin_meas:SUB Idlin_meas
1770 COM @Hp415x,@Form_off,INTEGER Hpib_sc,Swm
1780 COM /Meas_infol/ INTEGER Meas_points,Present,REAL Meas_str_time(*)
1790 COM /Meas_data1/ REAL Idlin_init,Idlin_shift(*)
1800 COM /Meas_data2/ REAL Gmmax_init,Gmmax_shift(*),Vtext_init,Vtext_shift(*)
1810 DIM Idvg$(100)
1820 REAL Idlin,Gmmax,Vtext
1830 !
1840 OUTPUT @Hp415x;":MMEM:LOAD:STAT 0,'MEM1.MES','MEMORY'"
1850 !
1860 OUTPUT @Hp415x;":PAGE:GLIS"
1870 OUTPUT @Hp415x;":DISP:WIND:STAT ON"
1880 OUTPUT @Hp415x;":PAGE:SCON:SING"
1890 OUTPUT @Hp415x;":*OPC?"
1900 ENTER @Hp415x;A
1910 !OUTPUT @Hp415x;":DISP:WIND:STAT OFF"
1920 OUTPUT @Hp415x;":TRAC? 'Idlin'"
1930 ENTER @Hp415x;Idlin
1940 OUTPUT @Hp415x;":TRAC? 'Gmmax'"
1950 ENTER @Hp415x;Gmmax
1960 OUTPUT @Hp415x;":TRAC? 'Vtext'"
1970 ENTER @Hp415x;Vtext
1980 IF Present=0 THEN
1990   Idlin_init=Idlin
2000   Gmmax_init=Gmmax
2010   Vtext_init=Vtext
2020   Idvg$=""IDVG0""
2030 ELSE
2040   Idlin_shift(Present)=Idlin
2050   Gmmax_shift(Present)=Gmmax
2060   Vtext_shift(Present)=Vtext
2070   Idvg$=""IDVG"&VAL$(Present)&""
2080 END IF
2090 OUTPUT @Hp415x;":PAGE:GLIS:LIST"

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```

2100 OUTPUT @Hp415x;":MMEM:STOR:SSH:DEL TAB"
2110 OUTPUT @Hp415x;":MMEM:STOR:SSH "&Idvg$
2120 OUTPUT @Hp415x;":*OPC?"
2130 ENTER @Hp415x;A
2140 SUBEND
2150 !
2160 Idsat_meas:SUB Idsat_meas
2170 COM @Hp415x,@Form_off,INTEGER Hpib_sc,Swm
2180 COM /Meas_infol/ INTEGER Meas_points,Present,REAL Meas_str_time(*)
2190 COM /Meas_data3/ REAL Idsat_init,Idsat_shift(*)
2200 REAL Idsat
2210 DIM Idvd$(100)
2220 !
2230 OUTPUT @Hp415x;":MMEM:LOAD:STAT 0,'MEM3.MES','MEMORY'"
2240 !
2250 OUTPUT @Hp415x;":PAGE:GLIS"
2260 OUTPUT @Hp415x;":DISP:WIND:STAT ON"
2270 OUTPUT @Hp415x;":PAGE:SCON:SING"
2280 OUTPUT @Hp415x;":*OPC?"
2290 ENTER @Hp415x;A
2300 !OUTPUT @Hp415x;":DISP:WIND:STAT OFF"
2310 OUTPUT @Hp415x;":TRAC? 'Idsat'"
2320 ENTER @Hp415x;Idsat
2330 IF Present=0 THEN
2340   Idsat_init=Idsat
2350   Idvd$="IDVD0"
2360 ELSE
2370   Idsat_shift(Present)=Idsat
2380   Idvd$="IDVD"&VAL$(Present)&""
2390 END IF
2400 OUTPUT @Hp415x;":PAGE:GLIS:LIST"
2410 OUTPUT @Hp415x;":MMEM:STOR:SSH:DEL TAB"
2420 OUTPUT @Hp415x;":MMEM:STOR:SSH "&Idvd$
2430 OUTPUT @Hp415x;":*OPC?"
2440 ENTER @Hp415x;A
2450 SUBEND
2460 !
2470 Stress:SUB Stress
2480 COM @Hp415x,@Form_off,INTEGER Hpib_sc,Swm
2490 COM /Meas_infol/ INTEGER Meas_points,Present,REAL Meas_str_time(*)
2500 REAL Duration,Acc_str
2510 !
2520 IF Present=1 THEN
2530   Duration=Meas_str_time(Present)
2540 ELSE
2550   Duration=Meas_str_time(Present)-Meas_str_time(Present-1)
2560 END IF
2570 OUTPUT @Hp415x;":PAGE:STR:SET:DUR "&VAL$(Duration)
2580 OUTPUT @Hp415x;":PAGE:SCON:STR"
2590 !
2600 OUTPUT @Hp415x;":*OPC?"
2610 ENTER @Hp415x;A
2620 SUBEND
2630 !
2640 Record_iddata:SUB Record_iddata
2650 COM @Hp415x,@Form_off,INTEGER Hpib_sc,Swm
2660 COM /File_name3/ Idlin_data$,Gmmax_data$,Vtext_data$

```


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```

2670 COM /Meas_info1/ INTEGER Meas_points,Present,REAL Meas_str_time(*)
2680 COM /Meas_info4/ INTEGER Gate_str,Source_str,Drain_str,Bulk_str
2690 COM /Meas_info5/ REAL Vdstr,Vgstr,Vdd,Vbb,Gate_length,Gate_width
2700 COM /Meas_data1/ REAL Idlin_init,Idlin_shift(*)
2710 DIM Idlin$(100)
2720 !
2730 ASSIGN @File TO Idlin_data$;FORMAT ON !Open the data file
2740 OUTPUT Idlin$ USING "DDDDDD.D,XXXXXXXX,SD.4DE,#";0,Idlin_init
2750 OUTPUT @File;Idlin$
2760 FOR Inc=1 TO Meas_points
2770   OUTPUT Idlin$ USING
"DDDDDD.D,XXXXXXXX,SD.4DE,#";Meas_str_time(Inc),Idlin_shift(Inc)
2780   OUTPUT @File;Idlin$
2790 NEXT Inc
2800 ASSIGN @File TO * !Close the file
2810 !
2820 CLEAR SCREEN
2830 OUTPUT @Hp415x;":DISP:WIND:ALL BST" ! Display IBASIC status screen
2840 !
2850 SUBEND
2860 Record_gmdata:SUB Record_gmdata
2870 COM @Hp415x,@Form_off,INTEGER Hpib_sc,Swm
2880 COM /File_name3/ Idlin_data$,Gmmax_data$,Vtext_data$
2890 COM /Meas_info1/ INTEGER Meas_points,Present,REAL Meas_str_time(*)
2900 COM /Meas_info4/ INTEGER Gate_str,Source_str,Drain_str,Bulk_str
2910 COM /Meas_info5/ REAL Vdstr,Vgstr,Vdd,Vbb,Gate_length,Gate_width
2920 COM /Meas_data1/ REAL Idlin_init,Idlin_shift(*)
2930 COM /Meas_data2/ REAL Gmmax_init,Gmmax_shift(*),Vtext_init,Vtext_shift(*)
2940 DIM Gmmax$(100)
2950 !
2960 ASSIGN @File TO Gmmax_data$;FORMAT ON !Open the data file
2970 OUTPUT Gmmax$ USING "DDDDDD.D,XXXXXXXX,SD.4DE,#";0,Gmmax_init
2980 OUTPUT @File;Gmmax$
2990 FOR Inc=1 TO Meas_points
3000   OUTPUT Gmmax$ USING
"DDDDDD.D,XXXXXXXX,SD.4DE,#";Meas_str_time(Inc),Gmmax_shift(Inc)
3010   OUTPUT @File;Gmmax$
3020 NEXT Inc
3030 ASSIGN @File TO * !Close the file
3040 CLEAR SCREEN
3050 OUTPUT @Hp415x;":DISP:WIND:ALL BST" ! Display IBASIC status screen
3060 !
3070 SUBEND
3080 Record_vtedata:SUB Record_vtedata
3090 COM @Hp415x,@Form_off,INTEGER Hpib_sc,Swm
3100 COM /File_name3/ Idlin_data$,Gmmax_data$,Vtext_data$
3110 COM /Meas_info1/ INTEGER Meas_points,Present,REAL Meas_str_time(*)
3120 COM /Meas_info4/ INTEGER Gate_str,Source_str,Drain_str,Bulk_str
3130 COM /Meas_info5/ REAL Vdstr,Vgstr,Vdd,Vbb,Gate_length,Gate_width
3140 COM /Meas_data1/ REAL Idlin_init,Idlin_shift(*)
3150 COM /Meas_data2/ REAL Gmmax_init,Gmmax_shift(*),Vtext_init,Vtext_shift(*)
3160 DIM Vth$(100)
3170 !
3180 ASSIGN @File TO Vtext_data$;FORMAT ON !Open the data file
3190 OUTPUT Vth$ USING "DDDDDD.D,XXXXXXXX,SD.4DE,#";0,Vtext_init
3200 OUTPUT @File;Vth$
3210 FOR Inc=1 TO Meas_points

```


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```

3220  OUTPUT Vth$ USING
"DDDDDD.D,XXXXXXX,SD.4DE,#";Meas_str_time(Inc),Vtext_shift(Inc)
3230  OUTPUT @File;Vth$
3240  NEXT Inc
3250  ASSIGN @File TO * !Close the file
3260  !
3270  CLEAR SCREEN
3280  OUTPUT @Hp415x;":DISP:WIND:ALL BST" ! Display IBASIC status screen
3290  !
3300  SUBEND
3310  Record_idsdata:SUB Record_idsdata
3320  COM @Hp415x,@Form_off,INTEGER Hpib_sc,Swm
3330  COM /File_name4/ Idsat_data$
3340  COM /Meas_info1/ INTEGER Meas_points,Present,REAL Meas_str_time(*)
3350  COM /Meas_info4/ INTEGER Gate_str,Source_str,Drain_str,Bulk_str
3360  COM /Meas_info5/ REAL Vdstr,Vgstr,Vdd,Vbb,Gate_length,Gate_width
3370  COM /Meas_data3/ REAL Idsat_init,Idsat_shift(*)
3380  DIM Idsat$[100]
3390  !
3400  ASSIGN @File1 TO Idsat_data$;FORMAT ON !Open the data file
3410  OUTPUT Idsat$ USING "DDDDDD.D,XXXXXXX,SD.4DE,#";0,Idsat_init
3420  OUTPUT @File1;Idsat$
3430  FOR Inc=1 TO Meas_points
3440  OUTPUT Idsat$ USING
"DDDDDD.D,XXXXXXX,SD.4DE,#";Meas_str_time(Inc),Idsat_shift(Inc)
3450  OUTPUT @File1;Idsat$
3460  NEXT Inc
3470  ASSIGN @File1 TO * !Close the file
3480  !
3490  CLEAR SCREEN
3500  OUTPUT @Hp415x;":DISP:WIND:ALL BST" ! Display IBASIC status screen
3510  !
3520  SUBEND

```

*****END OF PROGRAM*****

Appendix

QBasic Program for Dynamic NBTI_{inv} measurement:

```

100 !*****
110 !*
120 !* AC NBTI Stress/Masurement Test Using PGU1 to Gate electrode & PGU2 to Drain Electrode
130 !*
140 !* Edit History:
162 !* Created by Tan Shyue Seng on 27 Sep 2002
170 !*****
180 COM @Hp415x,@Form_off,INTEGER Hpib_sc,Swm
190 COM /File_name1/ Idlin_file$[12],Idsat_file$[12],Str_file$[12]
200 COM /File_name3/ Idlin_data$[100],Gmmax_data$[100],Vtext_data$[100]
210 COM /File_name4/ Idsat_data$[100]
220 COM /Meas_info1/ INTEGER Meas_points,Present,REAL Meas_str_time(1:30)
230 COM /Meas_info4/ INTEGER Gate_str,Source_str,Drain_str,Bulk_str
240 COM /Meas_info5/ REAL
Vdstr,Vgstr,Vganl,Pulse_period,Pulse_width,TrTime,Vdd,Vbb,Gate_length,Gate_width
250 COM /Meas_data1/ REAL Idlin_init,Idlin_shift(1:100)
260 COM /Meas_data2/ REAL Gmmax_init,Gmmax_shift(1:100),Vtext_init,Vtext_shift(1:100)
270 COM /Meas_data3/ REAL Idsat_init,Idsat_shift(1:100)
280 COM /Smu/ Vg$[4],Vs$[4],Vd$[4],Vb$[4]
290 !
300 ! ----- HP-IB Setup -----
310 INTEGER Hpib_addr,Swm_sc,Swm_addr
320 !
330 Hpib_sc=8      ! HP 415X HP-IB Select Code
340 Hpib_addr=0    ! HP 415X HP-IB Address
350 !
360 ASSIGN @Hp415x TO Hpib_sc*100+Hpib_addr
370 ASSIGN @Form_off TO Hpib_sc*100+Hpib_addr,FORMAT OFF
380 !
390 ! ----- Input Parameters -----
400 Vs$="SMU2"
410 Vg$="SMU1"
420 Vd$="SMU4"
430 Vb$="SMU3"
440 Meas_points=10    ! Number of times to repeat measurements
450 REDIM Meas_str_time(1:Meas_points)
460 REDIM Idlin_shift(1:Meas_points),Gmmax_shift(1:Meas_points),Vtext_shift(1:Meas_points)
470 REDIM Idsat_shift(1:Meas_points)
480 !
490 ! ----- Stress Condition for NBTI -----
500 Vdstr=0          ! Drain stress voltage
510 Vgstr=-2.6       ! Gate stress voltage (Pulse Base)
512 Vganl=0         ! Gate anneal voltage (Pulse Peak)
514 Pulse_freq=1000  ! AC Frequency (Hz)
520 Pulse_period=1/Pulse_freq
522 Pulse_width=Pulse_period*.5
530 TrTime=100E-9    ! Transistion Time
540 ! ----- Measurement Condition -----
545 Condition$="S18120002 W#16 18A"
546 Condition1$="Vg=Vd=-2.6V f=1KHz"
547 Condition2$="T=125C 10/0.12um"
548 Condition3$="Vdd=-1V "
549 Vdd=-1.0         ! Drain nominal voltage
550 Vbb=0            ! Bulk nominal voltage

```

Appendix

```

552 !
560 ! ----- Device geometries -----
570 Gate_length=1.2E-7 ! Gate length
580 Gate_width=1.0E-5 ! Gate width
590 !
600 ! ----- Definition of measurement and stress setup files -----
610 !
620 Str_file$="DNBTI3.STR" ! DC stress setup file
630 Idlin_file$="IDLIN.MES" ! Idlin/Gmmax/Vtext/Vtci measurement setup file
640 Idsat_file$="IDSAT.MES" ! Idsat measurement setup file
650 !
660 ! ----- File name to save ASCII data -----
670 Idlin_data$="IDLIN" ! Idlin shift data file name
680 Gmmax_data$="GM" ! Gmmax shift data file name
690 Vtext_data$="VTH" ! Vtext shift data file name
700 Idsat_data$="IDSAT" ! Idsat shift data file name
710 !
720 ! ----- Stress duration setup -----
730 Str_time: ! ! Stress duration data
740 DATA 2, 4, 10
742 DATA 20, 40, 100
744 DATA 200, 400, 1000
746 DATA 2000, 2001, 2002

780 RESTORE Str_time
790 READ Meas_str_time(*)
800 !
810 !////////// Main //////////
820 !
830 CALL Initial_setting ! Initial setting
840 CALL Init_hp415x ! Initialize HP 415X
850 CREATE Idlin_data$,100
860 CREATE Gmmax_data$,100
870 CREATE Vtext_data$,100
880 CREATE Idsat_data$,100
883 CREATE "Testcon",10
884 ASSIGN @File TO "Testcon";FORMAT ON
885 OUTPUT @File;Condition$
886 OUTPUT @File;Condition1$
887 OUTPUT @File;Condition2$
888 OUTPUT @File;Condition3$
889 ASSIGN @File TO *

890 ! --- Initial Characterization ---
900 Present=0
910 CALL Idsat_meas ! Initial Idsat characterization
920 CALL Idlin_meas ! Initial Idlin characterization
930 !CALL Record_iddata ! Record Idsat_shift data
940 !CALL Record_iddata ! Record Idlin_shift data
950 !CALL Record_gmdata ! Record Gmmax_shift data
960 !CALL Record_vtdata ! Record Vtext_shift data

970 !
980 ! ----- Stress/measurement cycle Characterization -----
990 FOR Present=1 TO Meas_points ! Start stress/measurement cycles
1000 CALL Stress ! Increment stress time and force stress
1010 CALL Idsat_meas ! Interim measurement

```


Appendix

```

1020 CALL Idlin_meas          ! Interim measurement
1030 NEXT Present
1040 CALL Record_idsdata     ! Record Idsat_shift data
1050 CALL Record_iddata      ! Record Idlin_shift data
1060 CALL Record_gmdata      ! Record Gmmax_shift data
1070 CALL Record_vtedata     ! Record Vtext_shift data
1080 DISP "NBTI Test is Completed!!"
1090 !
1100 END
1110 !!!!!!!!!!!!! Sub !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
1120 Initial_setting:SUB Initial_setting
1130 COM @Hp415x,@Form_off,INTEGER Hpib_sc,Swm
1140 COM /File_name1/ Idlin_file$[12],Idsat_file$[12],Str_file$[12]
1150 COM /File_name3/ Idlin_data$[100],Gmmax_data$[100],Vtext_data$[100]
1160 COM /File_name4/ Idsat_data$[100]
1170 COM /Meas_info1/ INTEGER Meas_points,Present,REAL Meas_str_time(*)
1180 COM /Meas_info4/ INTEGER Gate_str,Source_str,Drain_str,Bulk_str
1190 COM /Meas_info5/ REAL
Vdstr,Vgstr,Vganl,Pulse_period,Pulse_width,TrTime,Vdd,Vbb,Gate_length,Gate_width
1200 COM /Meas_data1/ REAL Idlin_init,Idlin_shift(*)
1210 COM /Meas_data2/ REAL Gmmax_init,Gmmax_shift(*),Vtext_init,Vtext_shift(*)
1220 COM /Meas_data3/ REAL Idsat_init,Idsat_shift(*)
1230 !
1240 COM /Smu/ Vg$,Vs$,Vd$,Vb$
1250 SUBEND
1260 Init_hp415x:SUB Init_hp415x
1270 COM @Hp415x,@Form_off,INTEGER Hpib_sc,Swm
1280 COM /File_name1/ Idlin_file$[12],Idsat_file$[12],Str_file$[12]
1290 COM /File_name3/ Idlin_data$[100],Gmmax_data$[100],Vtext_data$[100]
1300 COM /File_name4/ Idsat_data$[100]
1310 COM /Meas_info1/ INTEGER Meas_points,Present,REAL Meas_str_time(*)
1320 COM /Meas_data1/ REAL Idlin_init,Idlin_shift(*)
1330 COM /Meas_data2/ REAL Gmmax_init,Gmmax_shift(*),Vtext_init,Vtext_shift(*)
1340 COM /Meas_data3/ REAL Idsat_init,Idsat_shift(*)
1350 COM /Meas_info4/ INTEGER Gate_str,Source_str,Drain_str,Bulk_str
1360 COM /Meas_info5/ REAL
Vdstr,Vgstr,Vganl,Pulse_period,Pulse_width,TrTime,Vdd,Vbb,Gate_length,Gate_width
1370 COM /Smu/ Vg$[4],Vs$[4],Vd$[4],Vb$[4]
1380 !
1390 CLEAR SCREEN
1400 CLEAR @Hp415x
1410 OUTPUT @Hp415x;"*RST"          ! Device reset
1420 OUTPUT @Hp415x;"*CLS"          ! Clear status data
1430 OUTPUT @Hp415x;":STAT:PRES"    ! Preset event enable mask register
1440 OUTPUT @Hp415x;":DISP:WIND:STAT OFF" ! Screen update off
1450 OUTPUT @Hp415x;":CAL:AUTO OFF"  ! Auto calibration off
1460 OUTPUT @Hp415x;"*ESE 60;*SRE 32;*OPC?" ! Event status/service request enable register
setup
1470 ENTER @Hp415x:A
1480 OUTPUT @Hp415x;":DISP:WIND:ALL BST" ! Display IBASIC status screen
1485 OUTPUT @Hp415x;":PAGE:SCON:STAN ON" ! Standby ON
1490 !
1500 ! Load initial/interim characterization setup file into internal memory
1510 !
1520 OUTPUT @Hp415x;":MMEM:LOAD:STAT 0,'"&Idlin_file$&'",'DISK'"
1530 OUTPUT @Hp415x;":PAGE:MEAS:SWE:VAR1:STOP "&VAL$(Vdd)
1540 OUTPUT @Hp415x;":PAGE:MEAS:SWE:CONS:"&Vb$&" "&VAL$(Vbb)

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Appendix

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1541 !!!!!!! KEY IN Transistor Width and Length !!!!!!!
1542 OUTPUT @Hp415x;":PAGE:CHAN:UFUN:DEF 'W','um','10'"
1544 OUTPUT @Hp415x;":PAGE:CHAN:UFUN:DEF 'L','um','0.12'"
1546 OUTPUT @Hp415x;":PAGE:DISP:ANAL:MARK:POS 'ID','-0.1E-6*W/L'"
1550 OUTPUT @Hp415x;":MMEM:STOR:STAT 0,'MEM1.MES','MEMORY'"
1560 !OUTPUT @Hp415x;":MMEM:DEL ""&Idlin_file$&","'DISK',"
1570 !OUTPUT @Hp415x;":MMEM:STOR:STAT 0,""&Idlin_file$&","'DISK'"
1580 OUTPUT @Hp415x;":MMEM:LOAD:STAT 0,""&Idsat_file$&","'DISK'"
1590 OUTPUT @Hp415x;":PAGE:MEAS:SWE:VAR1:STOP "&VAL$(Vdd)
1600 OUTPUT @Hp415x;":PAGE:MEAS:SWE:CONS:"&Vb$&" "&VAL$(Vbb)
1610 OUTPUT @Hp415x;":MMEM:STOR:STAT 0,'MEM3.MES','MEMORY'"
1620 !OUTPUT @Hp415x;":MMEM:DEL ""&Idsat_file$&","'DISK',"
1630 !OUTPUT @Hp415x;":MMEM:STOR:STAT 0,""&Idsat_file$&","'DISK'"
1640 !
1650 ! Load stress setup file to HP 4155A/4156A
1660 !
1670 OUTPUT @Hp415x;":MMEM:LOAD:STAT 0,""&Str_file$&","'DISK'"
1672 OUTPUT @Hp415x;":PAGE:STR:SET:PULS:PGU1:PER ";Pulse_period
1674 OUTPUT @Hp415x;":PAGE:STR:SET:PULS:PGU1:WIDT ";Pulse_width
1680 OUTPUT @Hp415x;":PAGE:STR:SET:PULS:PGU1:LEAD ";TrTime
1682 OUTPUT @Hp415x;":PAGE:STR:SET:PULS:PGU1:TRA ";TrTime
1684 OUTPUT @Hp415x;":PAGE:STR:SET:PULS:PGU1:PEAK ";Vganl ! PGU1 pulse peak voltage
1686 OUTPUT @Hp415x;":PAGE:STR:SET:PULS:PGU1:BASE ";Vgstr ! PGU1 pulse base voltage
1687 OUTPUT @Hp415x;":PAGE:STR:SET:PULS:PGU1:IMP R50" ! Output impedance =50ohm to
prevent waveform overshoot
1688 OUTPUT @Hp415x;":PAGE:STR:SET:PULS:PGU2:PER ";Pulse_period
1690 OUTPUT @Hp415x;":PAGE:STR:SET:PULS:PGU2:WIDT ";Pulse_width
1692 OUTPUT @Hp415x;":PAGE:STR:SET:PULS:PGU2:LEAD ";TrTime
1694 OUTPUT @Hp415x;":PAGE:STR:SET:PULS:PGU2:TRA ";TrTime
1696 OUTPUT @Hp415x;":PAGE:STR:SET:PULS:PGU2:PEAK ";Vganl ! PGU2 pulse peak voltage
1700 OUTPUT @Hp415x;":PAGE:STR:SET:PULS:PGU2:BASE ";Vgstr ! PGU2 pulse base voltage
1702 OUTPUT @Hp415x;":PAGE:STR:SET:PULS:PGU2:DEL ";Pulse_width ! dELAY
1704 OUTPUT @Hp415x;":PAGE:STR:SET:PULS:PGU2:IMP R50" ! Output impedance =50ohm to
prevent waveform overshoot
1710 !OUTPUT @Hp415x;":MMEM:DEL ""&Str_file$&","'DISK'"
1720 !OUTPUT @Hp415x;":MMEM:STOR:STAT 0,""&Str_file$&","'DISK'"
1730 !
1740 SUBEND
1750 !
1760 Idlin_meas:SUB Idlin_meas
1770 COM @Hp415x,@Form_off,INTEGER Hpib_sc,Swm
1780 COM /Meas_info1/ INTEGER Meas_points,Present,REAL Meas_str_time(*)
1790 COM /Meas_data1/ REAL Idlin_init,Idlin_shift(*)
1800 COM /Meas_data2/ REAL Gmmax_init,Gmmax_shift(*),Vtext_init,Vtext_shift(*)
1810 DIM Idvg$(100)
1820 REAL Idlin,Gmmax,Vtext
1830 !
1840 OUTPUT @Hp415x;":MMEM:LOAD:STAT 0,'MEM1.MES','MEMORY'"
1850 !
1860 OUTPUT @Hp415x;":PAGE:GLIS"
1870 OUTPUT @Hp415x;":DISP:WIND:STAT ON"
1880 OUTPUT @Hp415x;":PAGE:SCON:SING"
1890 OUTPUT @Hp415x;""*OPC?"
1900 ENTER @Hp415x;A
1910 !OUTPUT @Hp415x;":DISP:WIND:STAT OFF"
1920 OUTPUT @Hp415x;":TRAC? 'Idlin'"
1930 ENTER @Hp415x;Idlin

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Appendix

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1940 OUTPUT @Hp415x;":TRAC? 'Gmmax'"
1950 ENTER @Hp415x;Gmmax
1960 OUTPUT @Hp415x;":TRAC? 'Vtext'"
1970 ENTER @Hp415x;Vtext
1980 IF Present=0 THEN
1990   Idlin_init=Idlin
2000   Gmmax_init=Gmmax
2010   Vtext_init=Vtext
2020   Idvg$="IDVG0"
2030 ELSE
2040   Idlin_shift(Present)=Idlin
2050   Gmmax_shift(Present)=Gmmax
2060   Vtext_shift(Present)=Vtext
2070   Idvg$="IDVG"&VAL$(Present)&""
2080 END IF
2090 OUTPUT @Hp415x;":PAGE:GLIS:LIST"
2100 OUTPUT @Hp415x;":MMEM:STOR:SSH:DEL TAB"
2110 OUTPUT @Hp415x;":MMEM:STOR:SSH "&Idvg$
2120 OUTPUT @Hp415x;"*OPC?"
2130 ENTER @Hp415x;A
2140 SUBEND
2150 !
2160 Idsat_meas:SUB Idsat_meas
2170 COM @Hp415x,@Form_off,INTEGER Hpib_sc,Swm
2180 COM /Meas_infol/ INTEGER Meas_points,Present,REAL Meas_str_time(*)
2190 COM /Meas_data3/ REAL Idsat_init,Idsat_shift(*)
2200 REAL Idsat
2210 DIM Idvd$(100)
2220 !
2230 OUTPUT @Hp415x;":MMEM:LOAD:STAT 0,'MEM3.MES','MEMORY'"
2240 !
2250 OUTPUT @Hp415x;":PAGE:GLIS"
2260 OUTPUT @Hp415x;":DISP:WIND:STAT ON"
2270 OUTPUT @Hp415x;":PAGE:SCON:SING"
2280 OUTPUT @Hp415x;"*OPC?"
2290 ENTER @Hp415x;A
2300 !OUTPUT @Hp415x;":DISP:WIND:STAT OFF"
2310 OUTPUT @Hp415x;":TRAC? 'Idsat'"
2320 ENTER @Hp415x;Idsat
2330 IF Present=0 THEN
2340   Idsat_init=Idsat
2350   Idvd$="IDVD0"
2360 ELSE
2370   Idsat_shift(Present)=Idsat
2380   Idvd$="IDVD"&VAL$(Present)&""
2390 END IF
2400 OUTPUT @Hp415x;":PAGE:GLIS:LIST"
2410 OUTPUT @Hp415x;":MMEM:STOR:SSH:DEL TAB"
2420 OUTPUT @Hp415x;":MMEM:STOR:SSH "&Idvd$
2430 OUTPUT @Hp415x;"*OPC?"
2440 ENTER @Hp415x;A
2450 SUBEND
2460 !
2470 Stress:SUB Stress
2480 COM @Hp415x,@Form_off,INTEGER Hpib_sc,Swm
2490 COM /Meas_infol/ INTEGER Meas_points,Present,REAL Meas_str_time(*)
2500 REAL Duration,Acc_str

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Appendix

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2510 !
2520 IF Present=1 THEN
2530   Duration=Meas_str_time(Present)
2540 ELSE
2550   Duration=Meas_str_time(Present)-Meas_str_time(Present-1)
2560 END IF
2570 OUTPUT @Hp415x;";PAGE:STR:SET:DUR "&VAL$ (Duration)
2584 OUTPUT @Hp415x;";PAGE:SCON:STR"
2590 !
2600 OUTPUT @Hp415x;"*OPC?"
2610 ENTER @Hp415x;A
2620 SUBEND
2630 !
2640 Record_iddata:SUB Record_iddata
2650 COM @Hp415x,@Form_off,INTEGER Hpib_sc,Swm
2660 COM /File_name3/ Idlin_data$,Gmmax_data$,Vtext_data$
2670 COM /Meas_info1/ INTEGER Meas_points,Present,REAL Meas_str_time(*)
2680 COM /Meas_info4/ INTEGER Gate_str,Source_str,Drain_str,Bulk_str
2690 COM /Meas_info5/ REAL
Vdstr,Vgstr,Vganl,Pulse_period,Pulse_width,TrTime,Vdd,Vbb,Gate_length,Gate_width
2700 COM /Meas_data1/ REAL Idlin_init,Idlin_shift(*)
2710 DIM Idlin$(100)
2720 !
2730 ASSIGN @File TO Idlin_data$;FORMAT ON !Open the data file
2740 OUTPUT Idlin$ USING "DDDDDD.D,XXXXXXXX,SD.4DE,#";0,Idlin_init
2750 OUTPUT @File;Idlin$
2760 FOR Inc=1 TO Meas_points
2770   OUTPUT Idlin$ USING
"DDDDDD.D,XXXXXXXX,SD.4DE,#";Meas_str_time(Inc),Idlin_shift(Inc)
2780   OUTPUT @File;Idlin$
2790 NEXT Inc
2800 ASSIGN @File TO * !Close the file
2810 !
2820 CLEAR SCREEN
2830 OUTPUT @Hp415x;";DISP:WIND:ALL BST" ! Display IBASIC status screen
2840 !
2850 SUBEND
2860 Record_gmdata:SUB Record_gmdata
2870 COM @Hp415x,@Form_off,INTEGER Hpib_sc,Swm
2880 COM /File_name3/ Idlin_data$,Gmmax_data$,Vtext_data$
2890 COM /Meas_info1/ INTEGER Meas_points,Present,REAL Meas_str_time(*)
2900 COM /Meas_info4/ INTEGER Gate_str,Source_str,Drain_str,Bulk_str
2910 COM /Meas_info5/ REAL
Vdstr,Vgstr,Vganl,Pulse_period,Pulse_width,TrTime,Vdd,Vbb,Gate_length,Gate_width
2920 COM /Meas_data1/ REAL Idlin_init,Idlin_shift(*)
2930 COM /Meas_data2/ REAL Gmmax_init,Gmmax_shift(*),Vtext_init,Vtext_shift(*)
2940 DIM Gmmax$(100)
2950 !
2960 ASSIGN @File TO Gmmax_data$;FORMAT ON !Open the data file
2970 OUTPUT Gmmax$ USING "DDDDDD.D,XXXXXXXX,SD.4DE,#";0,Gmmax_init
2980 OUTPUT @File;Gmmax$
2990 FOR Inc=1 TO Meas_points
3000   OUTPUT Gmmax$ USING
"DDDDDD.D,XXXXXXXX,SD.4DE,#";Meas_str_time(Inc),Gmmax_shift(Inc)
3010   OUTPUT @File;Gmmax$
3020 NEXT Inc
3030 ASSIGN @File TO * !Close the file

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Appendix

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3040 CLEAR SCREEN
3050 OUTPUT @Hp415x;":DISP:WIND:ALL BST" ! Display IBASIC status screen
3060 !
3070 SUBEND
3080 Record_vtedata:SUB Record_vtedata
3090 COM @Hp415x,@Form_off,INTEGER Hpib_sc,Swm
3100 COM /File_name3/ Idlin_data$,Gmmax_data$,Vtext_data$
3110 COM /Meas_info1/ INTEGER Meas_points,Present,REAL Meas_str_time(*)
3120 COM /Meas_info4/ INTEGER Gate_str,Source_str,Drain_str,Bulk_str
3130 COM /Meas_info5/ REAL
Vdstr,Vgstr,Vganl,Pulse_period,Pulse_width,TrTime,Vdd,Vbb,Gate_length,Gate_width
3140 COM /Meas_data1/ REAL Idlin_init,Idlin_shift(*)
3150 COM /Meas_data2/ REAL Gmmax_init,Gmmax_shift(*),Vtext_init,Vtext_shift(*)
3160 DIM Vth$[100]
3170 !
3180 ASSIGN @File TO Vtext_data$;FORMAT ON !Open the data file
3190 OUTPUT Vth$ USING "DDDDDD.D,XXXXXXXX,SD.4DE,#";0,Vtext_init
3200 OUTPUT @File;Vth$
3210 FOR Inc=1 TO Meas_points
3220 OUTPUT Vth$ USING
"DDDDDD.D,XXXXXXXX,SD.4DE,#";Meas_str_time(Inc),Vtext_shift(Inc)
3230 OUTPUT @File;Vth$
3240 NEXT Inc
3250 ASSIGN @File TO * !Close the file
3260 !
3270 CLEAR SCREEN
3280 OUTPUT @Hp415x;":DISP:WIND:ALL BST" ! Display IBASIC status screen
3290 !
3300 SUBEND
3310 Record_idsdata:SUB Record_idsdata
3320 COM @Hp415x,@Form_off,INTEGER Hpib_sc,Swm
3330 COM /File_name4/ Idsat_data$
3340 COM /Meas_info1/ INTEGER Meas_points,Present,REAL Meas_str_time(*)
3350 COM /Meas_info4/ INTEGER Gate_str,Source_str,Drain_str,Bulk_str
3360 COM /Meas_info5/ REAL
Vdstr,Vgstr,Vganl,Pulse_period,Pulse_width,TrTime,Vdd,Vbb,Gate_length,Gate_width
3370 COM /Meas_data3/ REAL Idsat_init,Idsat_shift(*)
3380 DIM Idsat$[100]
3390 !
3400 ASSIGN @File1 TO Idsat_data$;FORMAT ON !Open the data file
3410 OUTPUT Idsat$ USING "DDDDDD.D,XXXXXXXX,SD.4DE,#";0,Idsat_init
3420 OUTPUT @File1;Idsat$
3430 FOR Inc=1 TO Meas_points
3440 OUTPUT Idsat$ USING
"DDDDDD.D,XXXXXXXX,SD.4DE,#";Meas_str_time(Inc),Idsat_shift(Inc)
3450 OUTPUT @File1;Idsat$
3460 NEXT Inc
3470 ASSIGN @File1 TO * !Close the file
3480 !
3490 CLEAR SCREEN
3500 OUTPUT @Hp415x;":DISP:WIND:ALL BST" ! Display IBASIC status screen
3510 !
3520 SUBEND

```

*****END OF PROGRAM*****