RADIATION EFFECTS, NEGATIVE-BIAS-TEMPERATURE INSTABILITY, AND LOW-FREQUENCY $1/f$ NOISE IN SiGe/SiO$_2$/HfO$_2$ PMOS DEVICES

By

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Dissertation
Submitted to the Faculty of the
Graduate School of Vanderbilt University
in partial fulfillment of the requirements
for the degree of

DOCTOR OF PHILOSOPHY

in

Electrical Engineering
August, 2016
Nashville, Tennessee

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To My Wife and Kid,

With Love
ACKNOWLEDGEMENTS

I would like to first and foremost offer truly heartfelt thanks to my advisor Prof. Daniel M. Fleetwood for his invaluable guidance and support, and for pushing me to write this dissertation efficiently. It would be impossible to achieve my PhD degree without his help. It has always been a great pleasure for me working under his guidance for my PhD degree. He has always offered me professional guidance and shown me different ways to solve research problems. His profound knowledge and religious research attitude inspire me not only in the research but also in my life. I am lucky to have him as my advisor. I would also like to thank Prof. Ronald D. Schrimpf for sharing his knowledge through countless discussions when I encounter difficulties in research every Monday morning. I would also like to thank Professors Robert A. Reed and Sokrates T. Pantelides for serving on my oral and reading committee.

Many other people contributed to this work. I would like to especially thank Dr. Enxia Zhang. From the first day of my PhD research, Dr. Enxia Zhang stands out in teaching me how to use the experimental equipment and how to package the devices. Without her help, I would not perform my experiment. Then I would like to thank Jordan Hachtel who helped me get great STEM pictures of devices used in this work and collaborators from imec. I would also like to thank Xiao Shen for his DFT calculation to help explain the NBTI experimental data.

Finally a big thank you goes to my wife Dr. Cher Xuan Zhang for providing support for my work and in life.
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CHAPTER I

Introduction

For the past forty years, the performance of Metal-Oxide-Semiconductor Field-Effect Transistors (MOSFETs) has increased greatly after tremendously and aggressively scaling down the size of MOSFETs. The channel length and the gate oxide thickness are two of the major scaling parameters. During the last twenty years the gate length has been scaled down by a factor of over twenty, as shown in Fig. 1.1. At present, semiconductor companies have produced sub-22 nm gate length MOS transistors ahead of the roadmap in Fig. 1.1, and the physical channel length in these devices is typically shorter than the drawn length.

Fig. 1.1. MOS gate length trends and the 2011 International Technology Roadmap for Semiconductors (ITRS 2011) (after [1]).
The most widely accepted rule to keep transistors properly functioning is that both the supply voltages and dimensions are shrunk by the same factor in order to maintain an electric field in the small-sized device that is the same as for large devices. However, the thicknesses of conventional bulk SiO$_2$ gate dielectrics have reached the physical limitation (10-12 Å) [2], which is only a few atomic layers thick, due to the exponential increase in leakage current. To surmount this critical problem, high-permittivity (high-K) materials such as hafnium-based, zirconium and aluminum oxides [3] have been introduced as alternative gate dielectrics in place of the conventional SiO$_2$. High-K materials allow a further increase of the physical thickness of the gate stack to overcome the physical constrains and excessive leakage current, while keeping the equivalent oxide thickness (EOT) constant

\[
\text{EOT} = \frac{\varepsilon_{\text{high-K}}}{\varepsilon_{\text{SiO}_2}} d_{\text{high-K}},
\]

where $\varepsilon_{\text{SiO}_2}$ and $\varepsilon_{\text{high-K}}$ are the dielectric constant of silicon oxide and high-K material, respectively. $d_{\text{high-K}}$ is the physical thickness of high-K dielectric.

Not every high-K oxide can be a good substitute for SiO$_2$. Thermal Si oxide, which has been studied intensively for more than 40 years, forms an excellent interface with the Si. In addition to the high dielectric constant compared to SiO$_2$, there are several requirements for high-K materials that can be used as a MOS gate dielectric material. They must be thermodynamically stable with the Si channel and the gate electrode, and they should be kinetically stable and be compatible with processing to no less than 500 °C. Moreover, they should have band offsets with Si of over 1 eV so that the carrier injection into the oxide is minimized, have a high-quality interface with Si, and low bulk-oxide trap density. Table 1
summarizes various characteristics and main features of several alternative high-K gate dielectrics that were considered as potential materials for MOS gate dielectric applications.

Table 1. Comparison of the major characteristics, advantages, and disadvantages of existing and potential high-k gate dielectrics (After [3]).

<table>
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<tr>
<th>Dielectric</th>
<th>Dielectric constant (eV)</th>
<th>Bandgap (eV)</th>
<th>Conduction band offset (eV)</th>
<th>Merits</th>
<th>Drawbacks</th>
</tr>
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<tr>
<td>SiO$_2$</td>
<td>3.9</td>
<td>8.9</td>
<td>3.15</td>
<td>Excellent Si interface, low $Q_{ox}$ and $D_{it}$</td>
<td>Low-k</td>
</tr>
<tr>
<td>Si$_3$N$_4$</td>
<td>7-7.8</td>
<td>5.3</td>
<td>2.1</td>
<td>Good interface and bulk properties, medium $Q_{ox}$ and $D_{it}$</td>
<td>Low-k</td>
</tr>
<tr>
<td>Al$_2$O$_3$</td>
<td>9-10</td>
<td>8.8</td>
<td>2.8</td>
<td>$E_g$ comparable to SiO$_2$, amorphous</td>
<td>Medium $Q_{ox}$ and $D_{it}$, medium k</td>
</tr>
<tr>
<td>Ta$_2$O$_5$</td>
<td>25</td>
<td>4.4</td>
<td>0.36</td>
<td>High-K</td>
<td>Unacceptable $\Delta E_C$, not stable on Si</td>
</tr>
<tr>
<td>La$_2$O$_3$</td>
<td>~27</td>
<td>5.8</td>
<td>2.3</td>
<td>High-K, better thermal stability</td>
<td>Moisture absorption, unstable with Si</td>
</tr>
<tr>
<td>Y$_2$O$_3$</td>
<td>~15</td>
<td>6</td>
<td>2.3</td>
<td>Large $E_g$</td>
<td>Low crystallization temperature, high $D_{it}$, silicide formation</td>
</tr>
<tr>
<td>HfO$_2$</td>
<td>~20</td>
<td>5.6-5.7</td>
<td>1.3-1.5</td>
<td>Most suitable compared to other candidates</td>
<td>Crystallization, silicate and silicide formation</td>
</tr>
<tr>
<td>ZrO$_2$</td>
<td>~23</td>
<td>4.5-5.7</td>
<td>0.8-1.4</td>
<td>Similar to HfO$_2$</td>
<td>High $Q_{ox}$ and $D_{it}$, marginal stable with Si, crystallization, silicide formation</td>
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Among these, Hafnium oxide (HfO$_2$) and zirconium oxide (ZrO$_2$) are the materials with greatest potential to replace SiO$_2$ in MOS devices, mainly due to their relatively high dielectric constants compared to other high-K materials and better band offsets than most other high-K dielectrics, as shown in Fig. 1.2. HfO$_2$ is found to be thermodynamically stable when it forms an interfacial layer SiO$_2$ with Si, whereas the ZrO$_2$/Si interface is unstable [4]. The presence of a SiO$_2$ layer that is compatible with the Si substrate can separate the high-K oxide from the Si channel, which reduces the remote scattering caused by defects in high-K oxide. The stable interface with silicon makes HfO$_2$ a preferred candidate to replace SiO$_2$ as a gate dielectric over ZrO$_2$ [5],[6].

Fig. 1.2. Calculated conduction band and valence band offsets of various alternate oxides on Si (After [3]).

1.1 HfO$_2$

Atomic layer deposition (ALD) has emerged as an important technique for depositing thin high-K gate oxides in the MOSFET structure. However, the inefficient ALD nucleation is a very serious issue for the deposition of ultrathin high-K gate dielectric films. To grow an extremely uniform layer-by-layer ALD film, which is needed to ensure uniform electrical performance across the entire gate oxide, the nucleation of ALD precursors with the initial
surface species needs to be efficient on the very first ALD cycle. E. P. Gusev et al. [7] reported ultrathin hafnium oxide films deposited by ALD using sequential exposures of HfCl₄ and H₂O at 300 °C on a bare hydrogen-passivated silicon surface or a thin thermally grown SiO₂-based interlayer. High-resolution transmission electron microscopy (HRTEM) reveals that HfO₂ deposited on HF-last treated Si surfaces shows a non-uniform, island-like morphology and poor electrical properties due to inefficient nucleation on H-terminated Si as shown in Fig. 1.3(a). However, Fig. 1.3(b) captures a uniform HfO₂ ALD film on an ultrathin SiO₂ interlayer on the initial Si surface, which shows good electrical properties with respect to conventional SiO₂ gate dielectrics, which justifies its consideration as a candidate for high-K dielectric for MOSFETs. These comparison results highlight the important role of an ultrathin SiO₂ coating (< 1 nm) on Si in high surface qualities and electrical properties.

Fig. 1.3. HRTEM cross-section of a HfO₂ ALD film deposited on (a) a Si wafer immediately after HF-last surface treatment and (b) a SiO₂ layer on a Si wafer (after [7]).

G. Bersuker et al. [8] captured the oxygen removal from the underlying SiO₂ layer due to deposition and processing of the standard HfO₂ in electron spin resonance (ESR) spectra as shown in Fig. 1.4. The dominant electrically active defects at the Si/SiO₂ interface are Pₕ centers (Pₕ₀ and Pₕ₁, as will be discussed later), which involve an unpaired electron on a Si atom back bonded to three other Si atoms of the substrate at the Si/SiO₂ interface. The dominant defects in
the bulk SiO$_2$ observed here are E’ center defects, which consist of an unpaired electron on a Si atom back-bonded to three oxygen atoms. These E’ center defects are oxygen vacancies. Though the density of P$_b$ centers can be maintained at an acceptable level through hydrogen passivation, a potential consequence is that hydrogen could be released during device operation, under elevated temperature or under certain gate voltage conditions, thereby affecting device reliability.

Fig. 1.4. ESR spectra of the starting 1.1 nm SiO$_2$ layer, the same layer after ALD HfO$_2$ deposition, and after subsequent 1000 °C annealing (after [8]).

1.2 SiGe

In addition to the introduction of high-K material in MOS devices, the incorporation of several new materials and structural changes is required for continuing MOSFET evolution. The lattice constant of silicon is about 0.54 nm in a diamond cubic crystal structure [9]. The shorter the channel is, the easier it is to carry high currents. The key parameters are the inversion layer mobility and the density of charge in the inversion layer. People have been searching for alternative channel materials to replace silicon at the wafer surface, in an effort to improve the performance of MOS devices. Owing to the high hole mobility and compatibility with standard silicon processes, silicon germanium (SiGe) is of great interest as an alternative channel material.
to achieve a performance boost for $p$MOSFETs [10]. In July 2015, IBM announced that it made the advance by using SiGe instead of pure silicon in the first working sample of a chip with 7 nm transistors in the world. So SiGe is a promising candidate for the semiconductor industry at 7 nm nodes.

However, there are many issues that need to be solved for SiGe MOS devices. One of the significant issues concerning SiGe MOS fabrication is forming a stable interface between the gate dielectric and SiGe channel. Conventionally, a thin Si cap layer is used for SiGe surface passivation. The holes traveling in the SiGe channel are expected to have enhanced mobility by fundamentally altering the band structure of the channel due to the presence of the germanium. Furthermore, since the SiGe is separated from the gate oxide by a thin silicon cap layer, the surface scattering should be negligible. Q. Ouyang et. al. [11] proposed a novel $p$MOSFET with a SiGe S/D and a strained SiGe quantum well channel, as shown in Fig. 1.5. It has improved device performance and scalability to levels better as compared to those of a conventional Si $p$MOSFET.

![Fig. 1.5. Schematic diagram of a novel $p$MOSFET with a SiGe S/D, a Si cap layer and a strained SiGe quantum well channel (after [11]).](image-url)
1.3 Thesis Organization

It is necessary to evaluate the charge trapping characteristics and long-term reliability of SiGe/high-k structure devices for potential space-exploration applications. In this thesis, total-ionizing dose radiation effects, bias-temperature stress effects and low-frequency 1/f noise on SiGe/high-k structure are explored. This thesis is organized as follows: Chapter II goes over the basic mechanisms of total ionizing dose (TID) radiation effect and some popular models of negative bias temperature stability (NBTI) in pMOS. Chapter III introduces the background for analyzing noise in CMOS transistors. We review the basic mechanisms and models of 1/f noise in MOSFET transistors. Chapter IV focuses on the irradiation bias dependence of SiGe pMOS FinFETs as a function of total dose irradiation, and chapter V describes the negative bias temperature stress results on SiGe-pMOSFETs. Chapter VI presents and discusses experimental results on the temperature dependence of the 1/f noise on SiGe-pMOSFETs. Chapter VII concludes the thesis.
The first part of this chapter contains background information about total ionizing dose effects in MOS devices. The second part of this chapter describes the mechanisms of negative bias temperature instability (NBTI) in MOS devices. The midgap and subthreshold swing methods that are used in his work to separate the threshold voltage shifts due to oxide-trap charge ($\Delta V_{ot}$) and interface-trap charge ($\Delta V_{it}$) are described in detail.

2.1 Total ionizing dose effects in MOS devices

The microelectronic components in space are exposed to various types of radiation such as protons and electrons, which interact with the semiconductor material to cause ionizing damage, atomic displacement, and/or single event effects. Total-dose irradiation is a significant concern for the long-term reliability of MOS devices. It is extremely important to understand radiation effects on semiconductor devices for the application of advanced technologies and materials in space environments. This section will discuss the basic effects of radiation-induced charge buildup in MOS devices, including oxide, interface, and border traps.

Fig. 2.1 shows a schematic energy diagram of a MOS structure under positive bias applied to the gate and indicates four major physical processes that contribute to the radiation response of a MOS device. For MOS devices, the most total-dose radiation-sensitive parts are the oxide insulators. When a MOS device is exposed to high-energy ionizing radiation, electron-hole pairs are created in the oxide by the deposited energy (process 1). Because the electrons are much more mobile (20 cm$^2$/V sec at 300 K in fused quartz [12]) than the holes ($\sim 4 \times 10^{-9}$ cm$^2$/V
sec at 300 K) in SiO₂, most of the electrons are rapidly swept out of the oxide (within picoseconds), and holes are trapped in micro-structural defects and pre-existing traps. However, even before the electrons leave the oxide, some of the electrons will recombine with holes. The fraction of electron-hole pairs that escape recombination is called the charge yield. The fraction depends greatly on the strength of the electric field in the oxide and the energy of the incident particle. The generation and recombination of electron-hole pairs are the first processes shown in Fig 2.1. Those holes that escape initial recombination will further transport toward the Si/SiO₂ interface by hopping via localized states in the oxide (process 2) [13]. This process typically takes less than a second [14], but may take place over many decades in time. Because hole transport in SiO₂ is highly dispersive [15], as a result, the "tail" of the transport extends over several decades in time.

As the holes approach the Si/SiO₂ interface, some fraction of the holes are neutralized by electrons tunneling from silicon or thermal emission from the trap sites, and others get trapped at relatively deep trap states, forming positive oxide trap charges (process 3). These oxide trapped charges can cause a shift in the threshold voltage and an increase of radiation-induced leakage current (RILC) in these devices. RILC involves an inelastic tunneling process assisted by neutral traps in the oxide. The neutral electron trap likely originates as radiation-induced holes trapped at E’ centers (E’ centers will be described in detail later) in the oxide. The Electron Spin Resonance (ESR) measurements performed by P. M. Lenahan et al. have shown a link between E’ centers and RILC [17].

Meanwhile, hydrogen ions (protons) can be released in the oxide bulk as holes transport toward the interface through the oxide. Those protons can drift to the Si/SiO₂ interface under positive gate bias where they may react with Si-H to form H₂, leaving silicon dangling bonds at
the interface (process 4). These dangling bonds can act as interface traps, which are localized states in the Si band-gap. Their occupancy is determined by the Fermi level, leading to a change of threshold voltage and a decrease of carrier mobility.

Fig. 2.1. Schematic energy band diagram for MOS structure under positive bias, indicating major physical processes underlying radiation response. After [16].

As previously mentioned, some fraction of the radiation-induced holes will recombine with the electrons before the electrons are swept out of silicon dioxide, in a time on the order of a picosecond. The fraction of holes escaping initial recombination \( (f_h) \) depends strongly on the magnitude of the electric field through the oxide. When an electric field is applied across the oxide of a MOS device, the radiation-induced electron-hole pairs will immediately be separated and begin to transport in opposite directions. As the electric field strength increases to separate pairs more efficiently, the probability that a hole will recombine with an electron decreases, and the charge yield increases. Fig. 2.2 plots the fraction of holes that escape recombination for 10-keV x-ray irradiation as a function of the electric field. When the electric field is higher than 4 MV/cm, more than 80% of radiation-induced holes escape initial recombination.
In recent years, although manufacturers have been able to reduce EOT and increase physical oxide thickness by introducing high-K dielectric, the electric field present in the channel and gate dielectric has been increasing. Moreover, tunneling into the bulk high-K oxide increases as the interfacial SiO$_2$ oxide of the SiO$_2$/high-K dielectric stack composing the gate dielectric becomes thinner. As a result, operating temperatures have increased, too. Time-dependent dielectric breakdown (TDDB), hot carrier injection (HCI), and bias temperature instability (BTI) are three major reliability issues in modern CMOS technology. Among the three, BTI increases most sharply with electric field and temperature. BTI is a shift in threshold voltage with applied stress at elevated temperature. From the standpoint of lifetime of modern MOS transistors, the devices are considered to have failed when the shift exceeds typically 30 mV [19]. For highly scaled pMOSFETs, NBTI has been a more serious concern than positive BTI (PBTI). In 2014, J. H. Stathis et al. [19] showed operation voltage reduction requirement for gate oxide scaling at the 2014 IEEE Electron Device Meeting (IEDM) in Fig. 2.3. The 2013 ITRS roadmap anticipates sufficient voltage reduction to maintain nMOS scaling. However, NBTI may limit silicon-based pMOS scaling unless new materials such SiGe channel devices are adopted.
Fig. 2.3. Trend of maximum operation voltage $V_{\text{max}}$ for constant reliability for the three major gate dielectric failure modes, and ITRS roadmap trend for $V_{\text{dd}}$ and EOT scaling from 10nm node (after [19]).

2.2 What does NBTI do?

NBTI is associated with the creation of oxide charge and interface traps at the Si/oxide interface, when negative bias is applied to the gate at elevated temperatures. NBTI has a significant impact on pMOSFETs since these devices work under negative bias conditions during high-performance chip operation. Oxide-trapped charges are located within the oxide, and are not in electrical communication with the underlying Si. Interface traps are located at the Si/SiO$_2$ interface and in electrical communication with the underlying Si. Border traps are near-interfacial oxide traps that exchange charge with the underlying Si on the time scale of the measurements [20].

2.2.1 Oxide traps

There are a large number of oxygen vacancies close to the interface where oxidation is not complete. The oxygen vacancy can be activated into the paramagnetic state by irradiation or
electrical field stress. That radiation-induced or stress-induced paramagnetic center is termed an E’ defect, which is identified as a "trivalent silicon" back-bonded to three oxygen atoms in the oxide. There is one oxygen atom missing from the usual Si-O-Si lattice configuration, leaving a weak Si–Si bond. That an E’ center is an oxygen vacancy can be verified by ESR. J. T. Ryan et al. have observed that ESR spectra due to E’ center defects are generated by elevated temperature and modest negative gate bias and quickly disappear once the stress is removed [21].

E’ centers or oxygen vacancies are primarily responsible for hole traps in pMOS devices during NBTI. F. J. Feigl, W. B. Fowler and K. L. Yip proposed an oxygen vacancy model (Feigl-Fowler-Yip model) for the E’ center [22]. As illustrated in Fig. 2.4, after the hole is trapped in the precursor bridging-oxygen vacancy, a weak strained Si-Si bond configuration is broken. One of the Si atoms then relaxes back into a planar configuration, leaving it positively charged. The other Si remains neutral, with a dangling orbital containing one unpaired electron. An E’ center consists of these two trivalent Si atoms together. The E’ signal in ESR is actually obtained by resonant flipping of the spin of the unpaired electron on the neutral Si atom.

Fig. 2.4. Oxygen vacancy model for the E’ center in SiO₂. (a) Normal oxygen vacancy. An important feature is the existence of two inequivalent Si-O bonds. (b) Unrelaxed lattice oxygen vacancy. (c) Asymmetrically relaxed O⁻ vacancy (After [22]).
2.2.2 Interface traps

In addition to oxide traps, NBTI can also cause the formation of interface traps at the Si/SiO₂ interface. J. P. Campbell et al. [23] utilized spin-dependent recombination (SDR) to observe and identify two silicon dangling bond centers (P₁₀₀ and P₁₀₁ defects) at the Si/SiO₂ interface generated by a negative bias temperature in pMOSFETs. This P₀ center is also a “trivalent silicon” as is E’ center, but in this case the silicon is bonded to three Si atoms, with a dangling bond extending into the oxide, as schematically represented in Fig. 2.5. Because of the energy level within the Si bandgap and location at the interface, the interface defect is amphoteric, negatively charged above midgap, approximately neutral near midgap, and positively charged below midgap.

![Fig. 2.5. Schematic diagrams of P₁₀₀ and P₁₀₁ Si/SiO₂ interface traps (after [23]).](image)

Density functional theory calculations by Rashkeev et al. [24] strongly suggest that protons interact directly and break the Si-H bonds (P₀-H precursor sites) at the Si/SiO₂ interface via the simple reaction:

\[
H^+ + \text{Si-H} = \text{Si}^+ + \text{H}_2
\]

Fig. 2.6 traces the computed electric density contours in the region around a Si dangling bond passivated by hydrogen at the Si/SiO₂ interface during the depassivation process. The calculations suggest that two electrons leave the Si-H through Si-H-H⁺ bridge, forming a neutral H₂ molecule and leaving a dangling bond positively charged.
2.2.3 Border traps

A standard name for near-interfacial oxide traps that communicate with the Si was proposed as “border traps” by D. M. Fleetwood in 1992 [20]. Border traps are defined as near-interfacial oxide traps that are able to rapidly or slowly exchange charge with the underlying Si substrate over a very wide range of time scales. There is growing evidence that a large percentage of these defects are likely associated with E’ centers [20],[25],[26]. Border traps typically are located within a certain distance (~2 nm) in the oxide from the interface, as shown in Fig. 2.7.

Fig. 2.7. Schematic representation of (a) the physical location of oxide, interface, and border traps and (b) their electrical response (after [20]).
2.2.4 Charge separation techniques

To separate the effects of oxide and interface trap charge, the overall radiation response of a MOS device needs to be separated into its components:

\[ \Delta V_{th} = \Delta V_{ot} + \Delta V_{it} \]  \hspace{1cm} (2.1)

Here \( \Delta V_{ot} \) and \( \Delta V_{it} \) are the threshold voltage shifts due to oxide traps and interface traps, respectively. There are different methods for separating \( \Delta V_{th} \) into its components.

**Midgap charge separation method:**

The midgap charge separation method is based on the observation that the interface traps are approximately charge neutral for a device biased at midgap \([28],[29]\). The interface traps are amphoteric. In the upper portion of the band gap the interface traps are mostly acceptor-like. These are negatively charged when filled and neutral when empty. In the bottom portion of the band gap they are donor-like; these are neutral when filled and positively charged when empty, as shown in Fig. 2.8. In this case, the net oxide-trapped charge density changes can be estimated by the shifts in the midgap voltages \( \Delta V_{mg} \):

\[ \Delta V_{ot} = \Delta V_{mg} \]  \hspace{1cm} (2.2)

\[ \Delta V_{it} = \Delta V_{th} - \Delta V_{mg} \]  \hspace{1cm} (2.3)

Fig. 2.8. Band diagrams of the Si substrate of a p-channel MOS device showing the occupancy of interface traps and the various charge polarities with (a) negative interface trap charge at flatband and (b) positive interface trap charge at inversion (after \([30]\)).
The midgap voltages \( V_{mg} \) can be determined from subthreshold-current curves, as illustrated in Fig. 2.9. The interface trap charge density change \( \Delta N_{it} \) and oxide trap charge density change projected to the Si/SiO\(_2\) interface \( \Delta N_{ox} \) were estimated for MOS capacitors by the following equations:

\[
\Delta N_{ox} = -C_{ox} \frac{\Delta V_{mg}}{qA}
\]

\[
\Delta N_{it} = C_{ox} \frac{(\Delta V_{th} - \Delta V_{mg})}{qA}
\]

Here \( C_{ox} \) is the oxide capacitance, \(-q\) is the electronic charge, and \( A \) is the area.

Fig. 2.9. Subthreshold-current curves for an MOS transistor before and after irradiation (after [28]).

**Subthreshold swing method:**

The subthreshold technique is based on standard I-V characteristics [29]. When plotted as \( \log I_D \) versus \( V_G \), comparing the pre- and post-irradiation characteristics, the change in subthreshold swing, \( \Delta S \), can be determined. The subthreshold swing method of the charge separation technique is based on the calculation of the radiation induced voltage shift due to interface traps, \( \Delta V_{it} \), using the change subthreshold swing, \( \Delta S \):
\[ \Delta V_{it} = \frac{q \phi_s}{kT \ln 10} \Delta S, \]  
\[ \Delta V_{ot} = \Delta V_{th} - \Delta V_{it}, \]

(2.6)  (2.7)

Here \( \phi_s \) is the surface potential, \( k \) is Boltzmann's constant, and \( T \) is the absolute temperature.

### 2.3 How does NBTI work?

Although NBTI has been known for more than 30 years, the mechanism for NBTI is still under debate, only recently has a consensus begun to emerge. A number of mechanisms to explain NBTI have been proposed and discarded.

#### 2.3.1 Reaction-Diffusion model

NBTI has often been interpreted by some form of reaction-diffusion (RD) model, as originally proposed by Jeppson and Svensson [31]. The RD model is diffusion controlled and assumes that Si-H bonds at the semiconductor/oxide interface are broken at higher temperatures and electric fields, causing some hydrogen species to be released from previously passivated interface defects and then dispersively diffuse into the oxide.

Another RD model proposed by L. Tsetseris et al. [32] involves the depassivation of dopants in Si and subsequent movement of hydrogen species to the interface. First-principles calculations show that a direct depassivation reaction, \( \text{Si}_3=\text{SiH} + \text{H}^+ \rightarrow \text{Si}_3=\text{Si}^\bullet + \text{H}_2 \), is in fact possible. Here \( \text{Si}_3=\text{SiH} \) is a hydrogen-passivated interface trap and \( \text{Si}_3=\text{Si}^\bullet \) an interface trap with the dot representing the dangling bond. The hydrogen is assumed to be released from P-H bonds as the n-type Si surface is biased to depletion at elevated temperature. The hydrogen becomes positively charged (\( \text{H}^+ \)) by trapping a hole. \( \text{H}^+ \) is swept to the interface by the negative bias, and subsequently reacts with the Si-H bond to form \( \text{H}_2 \) leaving behind a positively charged Si dangling bond (or \( \text{P}_b \) center). The \( \text{H}_2 \) diffuses from the interface into the oxide.
However, recent studies of NBTI [33],[34] find that interface-trap creation is not the sole source of degradation but a major hole trapping effect also occurs, especially when electric fields during NBTI stress approaches or exceeds ~ 10 MV/cm. Additionally, a large number of detailed recovery studies published in the last decade [34],[35] cannot be fully accounted for by the reaction-diffusion mechanism family. As a consequence, recent research focus has shifted back toward charge trapping. Interestingly, this hole trapping mechanism was also suggested in the pioneering paper on the RD model by Jeppson and Svensson [31].

2.3.2 Two-stage model

In 2009 Grasser et al. developed a comprehensive quantitative two-stage model able to capture a large number of the features [36], suggesting the degradation is due to interface trap generation and/or oxide charge buildup. The degradation is assumed to proceed in two coupled stages. For the first stage, the NBTI degradation process is initiated (stage 1) when inversion layer hole capture occurs at an E’ precursor site, e.g., a neutral oxygen vacancy. The hole capture leads to positively charged E’ centers (paramagnetic defects observable with ESR) in the oxide, thereby creating a switching trap, as illustrated in Fig. 2.10. Upon hole capture, the Si–Si bond breaks and a positively charged E’γ center is created (state 2). Hole emission (electron capture) neutralizes the E’γ center (state 3). Being in state 3, two options exist: a hole can be captured again, causing a transition to state 2, or the structure can relax back to its equilibrium configuration (state 1). For the second stage, oxide silicon dangling bonds (E’ centers) created in the stage one process trigger the creation of Pb centers via hydrogen exchange with a Pb center at the interface. ESR measurements further confirmed that E’ centers are generated during NBTI stress and very quickly recover upon removal of the stress [21]. The E’ defect density does not change during zero oxide bias at elevated temperature or negative oxide bias at room temperature.
These observations support hole capture at an E’ precursor site and the creation of interface traps. Recently Grasser et al. [37]-[39] have also included hydrogen related centers associated with NBTI. Complexes incorporating oxygen and hydrogen (e.g., the hydrogen bridge, which is a hydrogen atom at a dimer O vacancy in SiO₂ [37]-[39], and the hydroxyl E’ center, a strained O bonded to a hydrogen atom [40],[41] may also affect NBTI. In contrast to the E’δ -centers, these defects are modified structurally and/or chemically via NBTI. Moreover, the hydrogen-related defects increase in density as a result of NBTI.

![Switching oxide trap model](image)

Fig. 2.10. Switching oxide trap model. After [36].
CHAPTER III

1/f noise theory

Many physical systems exhibit fluctuations with spectral densities that vary approximately as 1/f over a large range of frequencies. Several mechanisms exist that generate noise in semiconductors leading to a unique spectral power distribution in the frequency domain. Of these sources, the noise behavior of bulk CMOS devices is dominated primarily by two noise sources: thermal noise, flicker (1/f) noise. Other sources present in the noise spectrum include shot noise, generation/recombination (G-R) noise and random telegraph signal (RTS) noise. Fig. 3.1 shows a typical noise spectrum in a MOS transistor, in which the drain voltage power spectral density $S_V$ is plotted as a function of frequency, showing the dominance of 1/f noise at low frequencies and thermal noise at higher frequencies.

![Schematic variation of $S_V$ with frequency](image)

Fig. 3.1. Schematic variation of $S_V$ with frequency, showing the dominant 1/f noise at low frequencies, and dominant thermal noise at high frequencies (after [42]).

**Thermal noise:**

Thermal noise is intrinsic to all resistors and caused by the random thermal motion of charge carriers at any finite temperature. This noise is sometimes known as the Johnson-Nyquist
noise. The internal noise voltage source $V_t^2 (\text{V}^2)$ of the thermal noise across a resistor with resistance $R$ is described by the Nyquist equation [43],[44]:

$$V_t^2 = 4kTR\Delta f$$

(3.1)

Here $k$ is the Boltzmann constant, $T$ is the absolute temperature, and $\Delta f$ is the frequency bandwidth. $V_t^2$ depends on the temperature $T$, resistance $R$, and frequency $f$, but is independent of the current through the resistor. The voltage noise power spectral density of thermal noise $S_{Vt} (\text{V}^2/\text{Hz})$, $dV_t^2/df = 4kTR$, is independent of frequency. Thus, the thermal noise is the white noise.

3.1 Flicker noise

Flicker noise dominates the noise spectrum at low frequency. Flicker noise was first observed in vacuum tubes ninety years ago [45]. Flicker noise is also commonly called $1/f$ noise, because the noise spectrum varies as $1/f^\alpha$, where the exponent $\alpha$, $\frac{\partial \ln S_V}{\partial \ln f}$, is close to unity ($0.7 < \alpha < 1.3$). Here $S_V$ is the excess noise after the thermal noise $S_{Vt}$ is subtracted. $1/f$ noise is present in nearly all kinds of electronic devices under bias, including metal films, MOSFETs, BJTs, and diodes. A typical spectrum of $1/f$ noise in MOSFET with high-K gate dielectric stack is plotted in Fig. 3.2.

![Fig. 3.2. 1/f noise in TiN/HfO2/SiO2 pMOSFET biased at V$_{GS}$-V$_{th}$ = -0.6 V and V$_{DS}$ = -0.05 V and at T = 360 K.](image-url)
Although this noise is a nearly universal phenomenon in active devices, a variety of models have been proposed to explain 1/f noise in MOSFETs [46]-[48]. Two popular models have appeared in the literature to explain the occurrence of flicker noise in MOSFETs: the McWhorter number fluctuation theory and the Hooge mobility fluctuation theory. However, the thorough review of low-frequency 1/f noise by Fleetwood [49] shows a wealth of data demonstrating that the 1/f noise of semiconductor devices is due to carrier number fluctuations and not mobility fluctuations.

3.2 The McWhorter Model (Number Fluctuations)

In 1957, McWhorter proposed that flicker noise is primarily a surface effect. The McWhorter number fluctuation (ΔN) theory states that flicker noise is generated by fluctuations in the number of carriers due to charge trapping in surface states. McWhorter obtained the necessary 1/f spectrum by assuming that the time constant τ of the surface states varied with a 1/τ distribution. That is, 1/f characteristics superpose many different spectra of G-R noise, where free carriers are randomly trapped and trapped by trap centers with different life times. This was the basic concept behind the McWhorter model which assumed that: (a) trap centers are uniformly distributed in the silicon oxide near the silicon surface; (b) the carrier tunneling to trap centers decreases exponentially with the distance from the surface; (c) the time constants increase with the distance from the surface; and (d) separate centers involved in trapping/detrapping are independent.

A number of applications of the McWhorter theory to MOSFETs have been done. For example, the McWhorter model as adapted to MOS transistors enables one to obtain first-order estimates of effective trap densities for defects with energy levels that are reasonably close to the Si conduction band (for nMOS transistors) or valence band (for pMOS transistors), using the assumption that 1/f noise is associated with the capture and emission of charge carriers in the
conducting channel by trap sites in the oxide, at or near the Si/SiO$_2$ interface. In experiments the excess drain voltage noise power spectral density (PSD) with the devices operated in the linear region in strong inversion is measured. At strong inversion bias condition, drain voltage PSD can be expressed approximately as [50]:

$$S_{vd}(f, V_d, V_g) = \frac{K}{f^\alpha} \frac{V_d^2}{(V_g - V_t)^\beta}$$

(3.2)

where $\alpha$ and $\beta$ are fitting parameters that reflect the observed frequency dependence and gate-voltage dependence, respectively. $K$ is the normalized low-frequency $1/f$ noise magnitude as defined in Eq. (3.2). In the number fluctuation model that describes $1/f$ noise in MOSFETs:

$$K = \frac{q^2 k T D_{bt} t_{ox}^2}{L W e_{ox}^2 \ln(t_{max} / t_{min})}$$

(3.3)

Here $k$ is the Boltzmann constant, $T$ is the absolute temperature, $D_{bt}$ is the effective density of border traps per unit area per unit energy which can contribute to the $1/f$ noise process, $A$ is the channel surface area ($W \times L$), and $t_{max}$ and $t_{min}$ are presumed maximum and minimum “cutoff” times associated with the tunneling or thermally activated processes that lead to the observed noise.

In comparative studies with radiation effects, a strong correlation has been shown between the $1/f$ noise of MOS transistors and oxide-trap charge in SiO$_2$, whereas no correlation is generally observed between low frequency $1/f$ noise and interface-trap charge [50]-[52]. The $1/f$ noise of n-channel MOS devices increases with increasing oxide-trap charge during irradiation and decreases with decreasing oxide-trap charge during postirradiation annealing. Like hole trapping generated by negative bias-temperature stressing, the radiation-induced-hole trap was also identified as an E’ center introduced in chapter 2. So reducing the number of oxygen vacancies in the oxide can significantly reduce the $1/f$ noise of MOS devices.
3.3 The Dutta-Horn Model

The obvious candidates besides tunneling distances are activation energies. In 1979, Dutta, Dimon, and Horn [54] proposed that the nearly 1/f spectrum in metals was due to a broad distribution of activation energies. This technique was applied first to analyze the nearly 1/f spectrum noise in thin metal films, and then extend to Si- and compound-semiconductor-based microelectronic devices and materials.

Fig. 3.3. The distinction between the two energies: the energy difference between the states (ΔE) and thermal activation energy (E±)—for a two-level system in the classical regime (after [53]).

Dutta and Horn demonstrated that, if the noise is the result of thermally activated processes involving two energy levels separated by an energy barrier of $E_o$ that the system must overcome for the system to move from one configurational state to another [48],[53],[54], as shown in Fig. 3.3. A single two-state system can be characterized by two energies: the energy difference between the states, ΔE, and the thermal activation energy for making the transition, $E_o$ or $E^\pm$, which is inferred from the temperature dependence of the noise. In a collection of two-state systems defects have an energy distribution $D(E_o)$. The frequency exponent shows a temperature dependence described by:
\[
\alpha(\omega, T) = 1 - \frac{1}{\ln(\omega \tau_o)} \left( \frac{\partial \ln S_V(T)}{\partial \ln T} - 1 \right). 
\] (3.4)

Here

\[
\alpha = -\frac{\partial \ln S_V}{\partial \ln f}, 
\] (3.5)

\[
S_V \text{ is the excess voltage-noise power spectral density after the thermal noise is subtracted, and} \tau_o \text{ is the characteristic time of the process leading to the noise. For noise that is successfully described by Eq. (3.4), one can infer the shape of the defect-energy distribution } D(E_o) \text{ over a wide range of energies from noise measurements as a function of temperature } T \text{ via:}
\]

\[
D(E_o) \propto \frac{\omega}{kT} S_V(\omega, T) 
\] (3.6)

where the defect energy barrier is related to the temperature and frequency of the noise measurements through:

\[
E_o \approx -kT \ln(\omega \tau_o) 
\] (3.7)

In this work, low frequency 1/f noise measurements will be employed as a sensitive probe of defects that affect the devices threshold voltage and transconductance for SiGe pMOSFETs with HfO_2/SiO_2 gate oxide stack during NBTI.
Total ionizing dose irradiation responses of SiGe pMOS devices

This chapter explores the effects of 10-keV X-ray irradiation on SiGe pMOS FinFETs with a SiO$_2$/HfO$_2$/TiN gate stack under different irradiation biases. Negative threshold voltage shifts are observed in all cases, due to net positive oxide-trap charge. Negative bias irradiation leads to the worst-case degradation in the TID response of these devices. We attribute this to modification of the net trapped positive charge density in the HfO$_2$ layer as a result of additional radiation-induced holes that are generated in the SiO$_2$ interfacial layer of the bilayer insulating structure which, under negative bias, transport into and become trapped in the HfO$_2$. This leads to a more negative threshold voltage shift compared to 0 V irradiation. During positive bias irradiation, a number of radiation-induced electrons are generated in the SiO$_2$. These can similarly transport into and become trapped in the HfO$_2$, leading to a less negative threshold voltage shift than during 0 V irradiation.

4.1 Experimental details

pMOS FinFETs were fabricated on SOI wafers with strained Si$_{0.75}$Ge$_{0.25}$ fins that are intrinsically under ~1% compressive strain due to the lattice mismatch with the silicon buffer layer [55]. After the SiGe fin etching process, an HfO$_2$ layer (~2 nm) was formed by atomic layer deposition, and TiN and amorphous-Si were deposited. A ~1 nm SiO$_2$ interfacial layer (IL) was formed between the HfO$_2$ and SiGe fin, leading to an effective oxide thickness (EOT) of about 1.5 nm. Through this process, a high quality interface on SiGe can be achieved without the need for a Si cap layer [55]. This HfO$_2$/SiGe pMOS FinFET structure is shown schematically in Fig.
4.1(a). A TEM picture of the gate dielectric given in Fig. 4.1(b) clearly shows a SiO$_2$ interfacial layer existing between SiGe channel and HfO$_2$ dielectric. The work function difference between the TiN gate and SiGe is ~0.35 eV, as verified by Sentaurus device simulation [57]. The resulting structure has a built-in electric field of ~2MV/cm with 0 V applied bias.

![TEM picture of gate dielectric](image)

Fig. 4.1. (a) schematic and (b) TEM cross-section of a SiGe pMOS FinFET with HfO$_2$/SiO$_2$ gate dielectric (after [56]).

In this work, we have tested devices with a fin height ($H_{\text{fin}}$) of 40 nm and fin length ($L_{\text{fin}}$) of 250 nm. To examine the effects of the fin width ($W_{\text{fin}}$) on the TID response, two different as-drawn fin widths were measured: 50 and 100 nm. Although we follow the usual convention of quoting as-drawn fin widths in the descriptions of the experimental results that follow, the actual fin widths decrease with respect to the drawn width after device fabrication. In this case, the 50 nm drawn fin width is reduced to 25 nm in the fabricated device, while the 100 nm as-drawn fin-width is reduced to 70 nm. The presence of a hard mask on the top of the fin ensured double-gate instead of a trigate operation [55],[58]. The undoped Si layer that underlies the SiGe effectively decouples the device channel from the buried oxide [55],[58], consistent with the radiation response we report below.
Unlidded devices were irradiated at a dose rate of 31.5 krad(SiO$_2$)/min using a 10 keV ARACOR x-ray source, under positive, negative, and 0 V gate bias, with other terminals grounded, at room temperature. $I_D$-$V_G$ curves were measured to determine threshold voltage shifts ($\Delta V_{th}$), and components due to oxide-trap charge ($\Delta V_{ot}$) and effective interface-trap ($\Delta V_{it}$) density using the midgap charge separation technique as introduced in Chapter 2.2.4. We note that the effective interface-trap density most likely also includes contributions from fast border traps [59],[60]. Device characterization was performed in air with a HP 4156B Semiconductor Parameter Analyzer. During $I_D$-$V_G$ measurement, the source-drain voltage $V_{SD}$ was kept at 50 mV, while the gate voltage was swept from 0.5 V to $-1$ V. Stress-induced degradation without irradiation was also measured at comparable irradiation times and biases. All irradiations and electrical stresses and measurements were performed at room temperature. At least three devices were measured for each case.

4.2 Experimental results and discussion

Figs. 4.2(a) and (b) show the drain current $I_D$ at $V_{SD} = 50$ mV and transconductance $G_m$ versus gate voltage $V_G$ as a function of total dose at room temperature under negative and positive irradiation bias, respectively. The devices were irradiated up to 2 Mrad(SiO$_2$) at a gate bias of $-2$ V and $+1.5$ V, respectively, with all other terminals grounded. The $I_D$-$V_G$ curves shift negatively with total dose under both positive and negative gate bias, consistent with the buildup of net oxide-trap charge primarily in the HfO$_2$ dielectric layer [61]-[64], since no stable hole trapping is expected in the ultrathin SiO$_2$ layer [65]. No excess leakage due to charge trapping in the buried oxide is observed.
Fig. 4.2. Drain current $I_D$ and transconductance $G_m$ as a function of gate voltage $V_G$ and varying total dose with applied gate bias of (a) −2 V and (b) +1.5 V on devices of fin length/width ($W_{\text{fin}}/L_{\text{fin}}$) ratio = 50 nm/250 nm. The maximum effective mobility $g_{m,\text{max}}$ is degraded from ~352 (cm$^2$/V•s) to ~325 (cm$^2$/V•s) after 2 Mrad(SiO$_2$) irradiation under worst-case negative bias, as calculated via the equation $g_{m,\text{max}} = u_{\text{eff,}\text{max}}C_{\text{ox}}(W/L)V_{DS}$ in the non-saturated regime. Here $C_{\text{ox}} = 2.3$ μF/cm, effective gate width $W = 2 \times H_{\text{fin}} = 80$ nm, $L = 250$ nm, and $V_{DS} = 50$ mV (after [56]).
In Fig. 4.3, SiGe pMOS FinFETs are subjected to the same negative bias stress as in Fig. 4.2, with and without irradiation. The time scale on the top axis is matched to the time required for the total dose at the bottom axis for irradiation at a dose rate of 31.5 krad(SiO₂). The threshold voltage shift during negative gate bias is due to the tunneling of holes from the fin. The relatively large shifts at room temperature for high electric field indicate that shallow hole traps exist in the HfO₂ [63],[64]. In order to correct for the effect of the charge trapping that occurs as a result of electrical stress, adjusted values of purely radiation-induced $\Delta V_{th}$ (blue triangles) are obtained by subtracting $\Delta V_{th}$ due to negative bias stress without irradiation (black squares) from that due to negative-bias irradiation under negative bias (red circles).

Fig. 4.3 Threshold voltage shift due to negative-bias irradiation as a function of total dose and due to negative stress without irradiation as stress time on devices of fin length/width ($W_{fin}/L_{fin}$) ratio = 50 nm/250 nm (after [56]).

Fig. 4.4 shows the threshold voltage shifts as a function of total dose and corresponding stress times at an applied gate bias of +1.5 V for SiGe pMOS FinFETs with a HfO₂/SiO₂ gate
dielectric stack. No significant threshold voltage shifts are observed for these devices under similar stressing conditions for positive gate bias, without irradiation, indicating negligible stress-induced negative-charge trapping in the bulk of the HfO$_2$/SiO$_2$. The absence of electron trapping under positive bias stress is likely due to the presence of the interfacial layer SiO$_2$ which acts as an effective barrier for electron tunneling into HfO$_2$. Thus, we conclude that the threshold voltage shifts observed during positive bias X-ray exposure are only induced by the irradiation.

Fig. 4.4 $\Delta V_{th}$ as a function of dose for SiGe $p$MOS FinFETs irradiated with 10-keV X-rays at a dose rate of 31 krad(SiO$_2$)/min and as function of stress time without irradiation under +1.5 V (after [56]).

Fig. 4.5 shows the adjusted radiation responses of SiGe $p$MOS FinFETs irradiated with 10 keV X-rays up to 2 Mrad(SiO$_2$). The applied biases are +1.5 V for positive-bias irradiation and −2 V for negative-bias irradiation. Including the work function, the applied electric field for positive bias irradiation was ~ 12 MV/cm, 2 MV/cm for 0 V irradiation, and −11 MV/cm for negative bias irradiation. The largest threshold shift is observed for negative-bias irradiation, in contrast to what is typically observed for Si devices with SiO$_2$ or HfO$_2$ gate dielectrics [64].
Fig. 4.5 Adjusted $\Delta V_{th}$ as a function of dose under different irradiation bias conditions. The gate biases during irradiation are +1.5 V, 0 V, and –2 V (after [56]).

Fig. 4.6 Adjusted $\Delta V_{th}$ as a function of dose under different irradiation bias conditions for devices with 100 nm fin width and 250 nm fin length. The gate biases during irradiation are +1.5 V, 0 V, and –2 V (after [56]).

Fig. 4.6 plots the adjusted threshold shifts as a function of total dose for wide FinFETs having a gate length of 250 nm and fin width of 100 nm under the same bias conditions as for narrow FinFETs having a fin width of 50 nm. The negative bias configuration is again the worst-
case irradiation bias condition up to 2 Mrad(SiO$_2$). However, the threshold voltage shift (Fig. 4.6) for devices with a fin width of 100 nm is significantly larger than that of devices with 50 nm fin width (Fig. 4.5). That narrow fin devices exhibit reduced threshold voltage shifts as compared with wider fin devices in SOI FinFETs is commonly observed, which is usually attributed to the higher fringing electric fields and therefore enhanced charge yields that are observed in the wider fin devices [66],[67]. Given the already large applied electric fields in these devices, it seems unlikely that only fringing fields are responsible for the differences in Figs. 4.5 and 4.6, and differences in stress and therefore precursor defect density [68],[69] with fin width may be a more likely explanation. Despite the differences in overall charge trapping levels, the same relative differences are observed among the positive, 0 V, and negative bias irradiations, suggesting that these relative differences in response with applied bias are associated with differences in charge transport in the insulating layers of the gate stack.

4.3 Discussion

In Figs. 4.7(a) and (b), values of $\Delta V_{it}$ and $\Delta V_{ot}$ are plotted for the devices of Figs. 4.5 and 4.6, respectively. The largest shifts for both $\Delta V_{it}$ and $\Delta V_{ot}$ are observed for negative-bias irradiation. HfO$_2$ is known to trap both electrons and holes efficiently during radiation exposure and/or high-field stress [64],[70],[71]. We first considered that the differences in radiation response with bias could be caused by differences in charge trapping in the buried oxide, as is commonly the case for triple-gate FinFET devices [66],[72],[73]. However, as discussed above, these devices are designed and fabricated to minimize the effects of both the top and back channels on device operation [55],[58], consistent with the $I_D$-$V_G$ curves in Fig. 4.2. These show no back-channel leakage and very little subthreshold stretch-out, in contrast to devices with significant contributions from charge in the buried oxide to SOI FinFET radiation response.
This again suggests that charge transport effects in the insulating layers of the gate stack lead to the observed differences in radiation response with differences in applied bias.

Fig. 4.7. (a) $\Delta V_{it}$ and (b) $\Delta V_{ot}$ as a function of total dose for devices of fin length/width ($W_{fin}/L_{fin}$) ratio = 50 nm/250 nm at room temperature. The gate biases applied during irradiation are $+1.5$ V, 0 V and $-2$ V. The effective interface- and oxide-trap charge densities for 2 Mrad(SiO$_2$) irradiation under worst-case negative bias are $\sim 4 \times 10^{11}$ cm$^{-2}$ and $\sim 9 \times 10^{11}$ cm$^{-2}$ in (a) and (b), respectively (after [56]).
Fig. 4.8. Schematic energy-band diagram of a SiO$_2$/HfO$_2$/TiN gate stack under (a) −2 V and (b) +1.5 V gate bias. The radiation-induced electrons and holes can transport and become trapped in the defects located in the HfO$_2$ under electric field (after [56]).

The increase in net positive charge trapping in the negative bias case compared with the 0 V case suggests that the excess hole trapping observed during negative bias irradiation likely results from additional charge trapping in the HfO$_2$ due to radiation-induced holes that are generated in the SiO$_2$ and transport into the HfO$_2$. Similarly, during positive bias irradiation, radiation-induced electrons generated in the SiO$_2$ can transport into the HfO$_2$ and become trapped, leading instead to a less negative threshold voltage shift than observed for 0 V applied bias. This mechanism, depicted schematically in Fig. 4.8, and is consistent with the expected trapping responses of high-K dielectrics with relatively high electron and hole trap densities that overlie a SiO$_2$ layer with lower trapping densities [66],[70],[71]. It is also remarkably similar to the responses of thicker bilayer Si$_3$N$_4$/SiO$_2$ structures [74]-[76] that similarly pair an overlying material (Si$_3$N$_4$) that traps both electrons and holes efficiently with a SiO$_2$ layer with much lower trap density.
It is important to determine whether such a mechanism is plausible for these types of gate stacks with ultrathin SiO$_2$ layers. To do so, we estimate the percentage of radiation-induced electrons and holes $f_{e,h}$ generated in the ultrathin SiO$_2$ layer that would have to be trapped in the HfO$_2$ in Figs. 4.7 to account for the differences in response with radiation bias using the expression [77]:

$$f_{e,h} = \frac{\pm \Delta V_{e,h} \varepsilon_{ox}}{q\kappa_g f_y t_{ox} D}$$  \hspace{1cm} (4.1)

Here $\Delta V_{e,h}$ is the difference in threshold voltage shift due to excess electron or hole trapping as a result of the mechanism described above, $\varepsilon_{ox}$ is the dielectric constant of SiO$_2$, $-q$ is the electronic charge, $\kappa_g$ is the number of electron-hole pairs generated per unit dose in SiO$_2$ ($\sim 8.1 \times 10^{12}$ cm$^{-3}$ rad$^{-1}$ (SiO$_2$)), $f_y$ is the charge yield of SiO$_2$, $t_{ox}$ is the physical thickness of SiO$_2$ ($\sim 1$ nm), and $D$ is the total dose. We obtain first-order estimates of the values of $\Delta V_{e,h}$ by comparing the values of $\Delta V_{ot}$ at positive, negative, and 0 V bias in Figs. 4.5 and 4.6 for the narrow and wide fin width devices, respectively. Specifically, $\Delta V_e \approx (\Delta V_{ot})_{+1.5V \text{ bias}} - (\Delta V_{ot})_{0V \text{ bias}}$ and $\Delta V_h \approx (\Delta V_{ot})_{-2V \text{ bias}} - (\Delta V_{ot})_{0V \text{ bias}}$. The charge yield $f_y$ is estimated as $\sim 0.9$ in the SiO$_2$ at large positive or negative electric fields from [18]. The dose enhancement factor is estimated to be 2.5 for a thin SiO$_2$ layer surrounded by TiN, HfO$_2$, and Si from [78]. Applying these assumptions to the 2 Mrad(SiO$_2$) data in Figs. 4.5 and 4.6, we estimate an effective value of $(11 \pm 3)$% for $f_h$ and $(10 \pm 2)$% for $f_e$. These results are quite plausible when compared with trapping efficiencies observed in past studies of similar structures [79]. We emphasize that this calculation applies only to the differences in charge trapping that occur for different applied gate bias; a more comprehensive model of both positive and negative charge trapping would be required to characterize fully the electron and hole trapping in the insulating layers of these gate stacks, which is beyond the scope of the present study.
Finally, we note that the effective interface-trap buildup in these devices is smaller than the trapped-positive charge buildup, and is maximized for negative-bias irradiation. This suggests that the interface (or border) traps in these devices are not created via the release of hydrogen in the HfO$_2$ or SiO$_2$ layer, but may instead be due to hydrogen that is released from dopant atoms in the SiGe channel layer [80].

4.4 Summary of Chapter, and Conclusions

In this chapter, we report the irradiation and bias stress responses of SiGe $p$MOS FinFETs with HfO$_2$/SiO$_2$ gate dielectric stacks irradiated with 10 keV x-rays up to 2 Mrad(SiO$_2$). Experimental results suggest that negative bias irradiation leads to the worst-case degradation in the total dose response of SiGe $p$MOS FinFETs. We attribute this result to an increase in density of additional radiation-induced holes that become trapped in the HfO$_2$ under negative bias, and additional electron trapping under positive bias in the HfO$_2$, as compared with the 0 V irradiation case. A simple model of the structure suggests that these excess carriers originate in the near-interfacial SiO$_2$. 
CHAPTER V

Negative bias temperature instability responses of SiGe pMOS devices

In this chapter, we investigate negative-bias temperature instabilities in planar SiGe pMOSFETs with SiO$_2$/HfO$_2$ gate dielectrics. The measured activation energies for interface-trap charge buildup during negative bias-temperature stress are lower for SiGe channel pMOSFETs with SiO$_2$/HfO$_2$ gate dielectrics and Si capping layers than for conventional Si channel pMOSFETs with SiO$_2$ gate dielectrics. Electron energy loss spectroscopy and scanning transmission electron microscopy images demonstrate that Ge atoms can diffuse from the SiGe layer into the Si capping layer, which is adjacent to the SiO$_2$/HfO$_2$ gate dielectric. Density functional calculations show that these Ge atoms reduce the strength of nearby Si-H bonds, and that Ge-H bond energies are lower still, thereby reducing the activation energy for interface-trap generation for the SiGe devices. Activation energies for oxide-trap charge buildup during negative bias-temperature stress are similarly small for SiGe pMOSFETs with SiO$_2$/HfO$_2$ gate dielectrics and Si pMOSFETs with SiO$_2$ gate dielectrics, suggesting that in both cases the oxide-trap charge buildup likely is rate-limited by hole tunneling into the near-interfacial SiO$_2$.

5.1 Experimental details

The MOSFETs used in this work were provided by IMEC. The Si$_{0.55}$Ge$_{0.45}$ pMOSFETs were fabricated on an $n$-type Si wafer with a 4.0 nm Si$_{0.55}$Ge$_{0.45}$ layer deposited onto a 2.0 nm Si buffer. On top of the 1.4 nm Si capping layer, a ~2 nm HfO$_2$ layer and TiN metal gate were deposited. A cross sectional scanning transmission electron microscope (STEM) image of the fabricated SiGe pMOSFET with HfO$_2$/SiO$_2$ gate dielectric is shown in Fig 5.1(a) (All STEM
images shown in this thesis are obtained by Jordan Hatchtel at Oak Ridge National Laboratory). The 1.4 nm Si cap was partially oxidized, yielding a ~1 nm SiO$_2$ interfacial layer (IL) and an unconsumed 1.0 nm thick Si capping layer to passivate the Si$_{0.55}$Ge$_{0.45}$ surface and improve the interface quality. A higher resolution STEM cross-sectional image, depicted in Fig. 5.1(b), provides an atomistic picture of the Si-capped SiGe MOS structure and different atoms distribution from the Si substrate to TiN metal gate. Fig. 5.1(b) clearly shows both an amorphous SiO$_2$ layer (~1 nm) and the unconsumed, crystalline Si capping layer (~1 nm). No crystal lattice dislocations from the Si substrate through the Si capping layer are observed in either image, indicating that the Ge alloyed layer thickness (~4 nm) has not exceeded the critical relaxation thickness and that the SiGe channel is strained [82]. Due to the valence-band offset between SiGe and the Si cap (band diagram is shown in Fig 5.2), inversion holes are confined in the SiGe channel, which therefore acts as an implant free quantum well (IFQW). The equivalent oxide thickness (EOT) of the gate dielectric stack is about 1.5 nm. For comparison of the charge trapping properties, Si $p$MOS FinFETs with 2 nm SiO$_2$ gate dielectrics with fin width of 65 nm and fin length of 250 nm [72] were also measured.
Fig. 5.1. (a) STEM of the structural composition of the SiGe-on-Si MOS structure. (b) High resolution (5 nm) STEM cross-sections are shown for a SiGe pMOSFET with HfO$_2$/SiO$_2$ gate dielectric. The 1.4 nm Si cap was partially oxidized, yielding a ~1 nm SiO$_2$ interfacial layer and an unconsumed 1.0 nm thick Si capping layer (after [81]).

Fig. 5.2 Band diagram sketch of SiGe device (after [81]).
NBTI stress experiments were performed using the measure–stress–measure technique, as shown in Fig. 5.3. The Si\textsubscript{0.55}Ge\textsubscript{0.45} and Si devices were stressed at electric fields ($E_{ox}$) of approximately −11.1 MV/cm and −10.3 MV/cm in the SiO\textsubscript{2}, respectively (−2 V on the gate for the Si\textsubscript{0.55}Ge\textsubscript{0.45} devices, and −2.5 V for the Si devices). This ensures that the critical, near-interfacial SiO\textsubscript{2} layers in both the Si and SiGe devices have similar electric fields during stress. Devices were stressed at temperatures from 125 °C to 250 °C. Pre- and post-stress $I_D$-$V_G$ curves were measured after devices were cooled to room temperature. Pre- and post-stress $I_D$-$V_G$ curves were measured after devices were cooled to room temperature. Device characterization was performed in air with a HP 4156B Semiconductor Parameter Analyzer. During $I_D$-$V_G$ measurement, the source-drain voltage $V_{SD}$ was 50 mV, while the gate voltage was swept from 0.5 V to −1 V. At least five devices were measured for each case.

Fig. 5.3 NBTI experiment measurement flow chart.
5.2 Experimental Results and Analysis

Fig 5.4 (a) $I_D - V_G$ and (b) $G_m$ characterization as a function of gate voltage $V_G$ measured at room temperature for a 1 µm × 0.07 µm SiGe$_{0.45}$ pMOSFET after 30 min stress time. The stress bias is −2 V on the gate and the stress temperature is 150 °C (after [81]).
Fig. 5.4 shows the $I_D$-$V_G$ and transconductance $G_m$ characteristics as a function of gate voltage $V_G$ measured at room temperature before and after negative gate bias stress at -2 V. The $I_D$-$V_G$ curves shift negatively after 30 min of negative gate bias, and the peak $G_m$ is reduced with bias-temperature stress, which is due to the reduction of carrier mobility in the channel caused by charges trapped at (interface traps), or very close to (border traps), the Si/SiO$_2$ interface [59].

![Graph showing threshold voltage shift](image)

**Fig. 5.5** Threshold voltage shift $\Delta V_{th}$, as well as components due to oxide trap charge $\Delta V_{ot}$ and interface traps $\Delta V_{it}$, as a function of stress time for Si$_{0.55}$Ge$_{0.45}$ pMOSFETs with $W/L = 1$ µm/0.1 µm at 150 °C for $V_{stress} = -2$ V and $V_{relaxation} = 0$ V. The inset shows stress time exponents for $\Delta V_{th}$, $\Delta V_{ot}$, and $\Delta V_{it}$ (after [81]).

Threshold voltages due to oxide-trap $\Delta V_{ot}$ and effective interface-trap charge $\Delta V_{it}$, estimated via the subthreshold swing technique as introduced in Chapter 2.1.4, are shown as functions of stress and recovery time in Fig. 5.5. The threshold voltage shift is mainly due to oxide-trap charge, with a smaller contribution from interface traps. The effective interface-trap charge density likely also includes contributions from fast border traps [59],[60]. The inset of Fig. 5.5 shows that $V_{th}$ and its components due to oxide and interface trap charge have power law time $t$ dependences; the $t^{-0.21 \pm 0.02}$ time dependencies are similar to values observed for $\Delta V_{th}$ in previous work for Si/SiO$_2$/HfO$_2$/TiN structures [83].
Fig. 5.6. Arrhenius plots of effective (a) interface trap generation $\Delta N_{it} = -C_{ox} \Delta V_{it}/q$ and (b) oxide trap charge $\Delta N_{ot} = -C_{ox} \Delta V_{ot}/q$ densities for Si$_{0.55}$Ge$_{0.45}$ pMOSFETs with high-K dielectrics stressed at -11.1 MV/cm and for Si pMOSFETs with SiO$_2$ dielectric stressed at -10.3 MV/cm. Here $C_{ox}$ is the capacitance of oxide layer, and $q$ is the electronic charge. The SiGe devices with SiO$_2$/HfO$_2$ gate stacks show higher oxide-trap (~3x) and interface-trap (0.5 to 1.0x) charge densities than the Si devices with SiO$_2$ gate dielectrics, consistent with higher trap densities for devices with high-K gate stacks than with SiO$_2$ gate dielectrics (after [81]).
Fig. 5.6 shows changes of effective interface-trap and oxide-trap charge densities as functions of stress temperature for SiGe pMOSFETs and Si pMOS FinFETs. These devices were stressed with $-2 \text{ V}$ and $-2.5 \text{ V}$ on the gates, respectively. The activation energy values extracted from Arrhenius plots in Fig. 5.6(a) for effective interface-trap generation $E_{a,it}$ for the Si$_{0.55}$Ge$_{0.45}$ and Si pMOSFETs are 0.14 eV and 0.25 eV, respectively. The $E_{a,it}$ values for the Si pMOS FinFETs are similar to those reported for planar pMOS devices with SiO$_2$ gate dielectrics in the literature [84],[85]. The value of $E_a$ for the interface-trap buildup in the Si$_{0.55}$Ge$_{0.45}$ structures is 45% lower than the value for the Si/SiO$_2$ structure. Such a large percentage difference will lead to significant differences in estimates of long-term reliability under typical device operating conditions for these structures. In contrast, the extracted activation energy for oxide-trap charge $E_{a,ot}$ is 0.13 eV for the Si$_{0.55}$Ge$_{0.45}$ pMOSFETs and 0.16 eV for the Si pMOSFETs, as shown in Fig. 5.6(b). Moreover, the SiGe device with the SiO$_2$/HfO$_2$ gate stack shows both higher oxide-trap (~3x) and effective interface-trap charge densities than the Si device with the SiO$_2$ dielectric. Higher trapped charge densities are observed, as expected, for devices with high-K gate stacks than for devices with SiO$_2$ gate dielectrics. Note that incorporation of Ge into the channel can significantly reduce NBTI degradation for devices with high-K gate dielectrics [86].

Similarly small activation energies for oxide-trap charge indicate that both cases likely are dominated by hole tunneling into defects (oxygen vacancies) in the near-interfacial SiO$_2$ and HfO$_2$ [87],[88], although a role for H$^+$ trapping [32] cannot be ruled out. Fig. 5.7 shows the band diagram for negative gate bias, including pre-existing oxygen vacancy energy levels in the near-interfacial SiO$_2$ and HfO$_2$ layers. In both structures, under high electric field conditions, holes from the channel tunnel into oxygen vacancies in the near-interfacial SiO$_2$. In SiO$_2$ devices, holes are trapped in $E'$ defects (O vacancies) [21],[23],[32],[88]. The weak temperature dependence
and the similarities of the activation energies for the two types of structures in Fig. 5.6(b) suggest that the hole injection into the near-interfacial SiO$_2$ via tunneling is most likely the rate limiting step in this process, since the energy levels of defects in HfO$_2$ and SiO$_2$ are quite different, in general [70],[90]. In the Si$_{0.55}$Ge$_{0.45}$ pMOSFETs, holes that would otherwise transport across the ultrathin SiO$_2$ without becoming trapped may instead become trapped in the HfO$_2$ [86],[88]. This will lead to a more negative shift in threshold voltage, but similar trapping kinetics, as long as hole injection is the rate limiting step in each case.

![Fig. 5.7. Schematic diagram for negative gate bias in SiGe pMOSFETs, including different defect bands associated with oxygen vacancies in the interfacial layer and HfO$_2$ (after [70],[86]).](image)

It has been shown that the interface trap generation observed at measuring times comparable to those in this work in Si MOS transistors during NBT stress is governed by the depassivation of interface Si-H bonds [85]. Tsetseris et al. [32] performed density functional calculations which showed that Si-H bonds cannot be broken by direct hole capture from the
substrate. However, these bonds can be broken through direct reaction with protons
\[(\text{Si} - \text{H} + \text{H}^+ \rightarrow \text{Si}^+ + \text{H}_2)\]
that are released from dopants in the semiconductor and drift under negative bias toward the semiconductor-dielectric interface [32],[91]. Here Si\(^+\) denotes a positively charged Si dangling bond. At temperatures above 100 °C, the balance of the reaction is controlled by the diffusion of the product H\(_2\). The activation energy \(E_a\) for interface trap generation is
\[E_a = \frac{1}{2} \Delta E + \frac{1}{4} \phi_D,\]
where \(\Delta E\) is the reaction energy of the depassivation process and \(\phi_D\) is the diffusion barrier of H\(_2\) in SiO\(_2\) [32],[91],[92]. Assuming the diffusion barrier of H\(_2\) in SiO\(_2\) is the same in the Si capped SiGe MOS and Si MOS structures, the 0.11 eV difference in the \(E_a\) for interface trap generation, as shown in Fig. 5.6(a), suggests that, on average, the reaction energy \(\Delta E\) for the Si capped SiGe MOS structure is 0.22 eV lower than that for the Si MOS structure. As shown below, this reduction of reaction energy occurs because Ge atoms are present in the Si capping layer.

STEM provides an atomistic picture of the Si-capped SiGe MOS structure and Ge distribution. Annular bright field (ABF) and high angle annular dark field (HAADF) images obtained using an aberration-corrected STEM operating at 200 kV are shown in Figs. 5.8(a) and (b), which clearly show both an amorphous SiO\(_2\) layer (~1 nm) and the unconsumed, crystalline Si capping layer (~1 nm). No crystal lattice dislocations from the Si substrate through the Si capping layer are observed in either image, indicating that the Ge alloyed layer thickness (~4 nm) has not exceeded the critical relaxation thickness and that the SiGe channel is strained [82]. Aligning two-dimensional spectral images of the chemical concentrations of O, Ge, and Si and their integrated intensities obtained via electron energy loss spectroscopy (EELS) with the STEM images, as shown in Figs. 5.8(c)-(f), we can determine the chemical content in each layer. Figs.
5.8(d) and (f) both a strong Ge EELS signal throughout the capping layer and partially within the oxide layer, confirming a significant amount of Ge diffusion into the cap during device processing [93].

![Scanning transmission electron microscope analysis of structural composition. Annular (a) bright and (b) dark field images of the structure. The lack of interfacial misfit dislocations shows that the crystal lattices in the channel and capping layer have not expanded due to the Ge, but are instead strained. Two dimensional elemental maps of the device are shown in (c)-(e). The electron energy loss spectra (EELS) for O (c), Ge (d), and Si (e) are shown across same regions in (a) and (b). The EELS intensities from (c)-(e) are vertically summed in (f), normalized to the maximum value for each element, and then plotted jointly. There is significant Ge diffusion into the Si capping layer, all the way up to the oxide layer (after [81]).]
Density functional calculations [94] show that, on the hydrogenated SiGe surface, the presence of Ge can reduce the reaction energy and barrier of hydrogen desorption from the surface. Here we evaluate the effects of near-interface Ge on the reaction energy $\Delta E$ of hydrogen depassivation ($\text{Si} - \text{H} + \text{H}^+ \rightarrow \text{Si}^+ + \text{H}_2$) at the Si/SiO$_2$ interface. The calculations were done by Xiao Shen who was from Department of Physics and Astronomy at Vanderbilt University and now an associate professor in University of Memphis using an interface model of a $(2\sqrt{2} \times 2\sqrt{2})$ unit cell of Si (100) surface constructed by a Monte-Carlo bond-switching method [95]. The model consists of a slab of crystalline Si with a thickness of 17 Å and an amorphous SiO$_2$ layer with a thickness of 13 Å. At the interface, there is one Si dangling bond passivated by a H atom, as shown in Fig. 5.9(a). The calculations use the Perdew-Burke-Ernzerhof (PBE) [96] version of exchange-correlation functional, projector augmented wave (PAW) potentials [97], and planewave basis as implemented in the VASP (Vienna ab initio simulation package) code [98]. The planewave kinetic energy cutoff is 283 eV. The structural relaxations are converged to $10^{-3}$ eV for the total energy difference between two ionic steps. A single k-point at (0.25, 0.25, 0.25) is used for Brillouin zone sampling.

We first compute the reaction energy $\Delta E$ at the Si/SiO$_2$ interface without Ge, as shown in Fig. 5.9(a). The initial and final states of the reaction are shown in Figs. 5.9(b) and 4.9(c). A reaction energy $\Delta E$ of 0.44 eV is obtained, which is in good agreement with the value of 0.5 eV from a previous study [99]. Calculations show that, when the Si atom in the Si-H bond has a Ge neighbor, as shown in Fig. 5.9(d), the reaction energy $\Delta E$ is reduced by 0.10 eV. When the Ge atom replaces the Si atom in Si-H bond, as shown in Fig. 5.9(e), the reaction energy $\Delta E$ is reduced by 0.51 eV and becomes negative. The large reduction of reaction energy for depassivating a Ge-H bond compared to a Si-H bond suggests that having Ge exposed near the
interface can pose potentially significant reliability concerns, which highlights the importance of the Si capping layer employed in these devices. The observed reduction of 0.22 eV in $\Delta E$ (0.11 eV in $E_a$) is likely the averaged value of depassivation from a majority of Si-H bonds with Ge neighbors and from a small number of Ge-H bonds directly at the interface.

Fig. 5.9. Models of the Si/SiO$_2$ interface for calculating the reaction energies (blue: Si, red: O, white: H, grey: Ge): (a) an interface model with an Si-H bond; (b) the initial configuration of the depassivation reaction with an H$^+$ at the vicinity of the Si-H bond; (c) the final configuration of the depassivation reaction with a H$_2$ molecule and a Si dangling bond; (d) an interface model with an Si-H bond similar to (a), with the Si atom in the Si-H bond having a Ge neighbor; (e) an interface model similar to (a), with a Ge atom replacing the Si atom in Si-H bond (after [81]).

5.3 Conclusion of Chapter

In summary, positive oxide-trap charge trapping is the dominant defect responsible for NBTI in Si$_{0.55}$Ge$_{0.45}$ pMOSFETs with high-K dielectrics. The experimental results show similarly small values of $E_a$ for oxide-trap charge buildup, while $E_a$ is lower for interface-trap buildup in the pMOSFETs with Si$_{0.55}$Ge$_{0.45}$ channel and high-K gate stacks, compared to the Si channel devices with SiO$_2$ gate dielectrics. The similar activation energies for oxide-trap charge
in these two structures suggests that hole injection into the near-interfacial SiO$_2$ via tunneling is evidently the rate-limiting process for oxide-trap charge buildup during negative-bias stress. Electron energy loss spectroscopy shows the presence of Ge atoms in the Si capping layer. First-principles calculations show that Ge atoms near the Si/SiO$_2$ interface are primarily responsible for the reduced activation energies for interface traps in the SiGe $p$MOS devices, as compared with the Si $p$MOS devices.
CHAPTER VI

Low-frequency 1/f noise in SiGe pMOSFETs

This chapter explores the low-frequency 1/f noise on Si$_{0.55}$Ge$_{0.45}$ pMOSFETs with a SiO$_2$/HfO$_2$/TiN gate stack. Low-frequency 1/f noise measurements can provide insight into the density and energy distributions of defects in gate dielectrics in a wide range of applications [49],[50],[100]-[104]. It has been demonstrated that the 1/f noise of pMOS devices with SiO$_2$, oxynitride, and/or high-K dielectric layers increase with negative-bias-temperature stress [104]-[110]. To date, most of these noise measurements have been performed at room temperature, which limits the amount of information that can be obtained about defect densities and energies to a narrow range of energy levels. In our experiment, we extend the available temperature range from 100 K to 450 K, which is essentially the regular operation temperature of MOS transistors, corresponding to 0.26 eV to 1.13 eV of observable energy window contributing to NBTI. Fig. 6.1 shows low-frequency 1/f noise measurements as a function of temperature (100-440 K) for devices with or without negative-bias-temperature stress (NBTS) for Si$_{0.55}$Ge$_{0.45}$ pMOSFETs with a Si capping layer and SiO$_2$/HfO$_2$/TiN gate stack. Clearly, the lower-temperature noise is relatively unchanged by NBTS, but the higher-temperature noise is changed significantly. In this chapter, we describe the devices, experimental test conditions, and analysis of a series of experiments that were performed to obtain insight into the underlying defects responsible for the device degradation and increased low-frequency noise in these devices. The results suggest a significant role for hydrogen-related defects in the near-interfacial SiO$_2$/HfO$_2$ dielectric layers, and provide insight into the densities and energy levels of these defects.
Fig. 6.1. Noise magnitude $S_{vd}$ at $f = 10$ Hz as a function of temperature from 100 K to 440 K for a SiGe $p$MOSFET with a Si capping layer and SiO$_2$/HfO$_2$ gate dielectric. The stressed device was held at a constant gate bias of -2 V for ~ 10 min at each successively higher temperature before noise measurements were performed. The unstressed device was held with all pins grounded for a similar amount of time at each successively higher temperature. During the noise measurement, the transistor was biased at $V_D = -50$ mV and $V_{GS-Vth} = -0.6$ V.

### 6.1 Experimental Details

The information on devices used in the noise measurement refers to that in Chapter 4.1. Figs. 5.8(c) and 3(f) both show a weak oxygen EELS signal throughout the interfacial layer SiO$_2$ and at the SiO$_2$/HfO$_2$ interface, confirming a relatively high density of oxygen vacancies in those regions. The wafers were first diced to individual dies. Then the diced die, containing the isolated SiGe $p$MOSFETs, was mounted on a high speed package which has a good contact with the stage of bonder. The package, mounting the device under study (DUT), was removed from the stage and put in an electro-static discharge (ESD) proof box every time when the bonder needs to generate a ball at the tip of gold wire by sparkling. This was to ensure the survival of devices from possible transient spikes or ESD during sparking. A grounded wrist strap was
always used while handling the devices.

Packaged Si$_{0.55}$Ge$_{0.45}$ devices were stressed at electric fields ($E_{ox}$) of approximately $-11.1$ MV/cm in the SiO$_2$ ($-2$ V on the gate) for fixed duration of 10 min at temperatures from 100 K to 440 K in a vacuum cryostat with an automatic temperature controller. $I_D$-$V_G$ curves were measured before and 5 min after stress to allow recovery of the fast component of negative-bias-temperature instability (NBTI), so that NBTI degradation remains almost constant during $I_D$-$V_G$ and $1/f$ noise measurements. Device DC characterization was performed in vacuum with a HP 4156B Semiconductor Parameter Analyzer. During $I_D$-$V_G$ measurement, the source-drain voltage $V_{SD}$ was $-50$ mV, while the gate voltage was swept from $0.5$ V to $-1$ V. Low frequency $1/f$ noise measurements were performed in the linear mode of device operation using the setup in Fig. 6.2 [111], before and after NBTI stress.

![Diagram](image.png)

Fig. 6.2. Low frequency $1/f$ noise measurement setup. (After Xiong et al. [111].)

### 6.2 Experimental Results and Analysis

#### 6.2.1 Temperature dependence of $1/f$ noise without stress

Drain voltage noise power spectral densities ($V^2$/Hz) for a SiGe $p$MOSFET with a gate width $W = 1$ μm and gate length $L = 0.47$ μm were measured from 100 K to 440 K in steps of 10
K. During the noise measurement, the transistor was biased in the linear mode of device operation at each temperature with constant $V_D = -50$ mV and $V_{GS-V_{th}} = -0.6$ V. Fig. 6.3 shows the PSD of signal noise measured at -50 mV drain bias and background noise measured at 0 V drain bias at 300 K. The background noise is usually caused by thermal noise and shot noise. Fig. 6.4 shows excess noise $S_{vd}$ spectra with the background noise subtracted at different temperatures. The inset of Fig. 6.4 shows the threshold voltage of an unstressed device as a function of temperature. The threshold voltage was measured from the $I_D-V_G$ curve at each temperature to ensure that $V_{GS-V_{th}}$ was held constant for all noise measurements, to ensure a constant surface potential. We fit excess $S_{vd}$ curves similar to those in Fig. 6.4 for $f = 5$ Hz to 40 Hz to extract the frequency exponent $\alpha$ (Eqs. (3.5)), as well as the value of $\partial \log S_{vd}/\partial \log f$ (Eq. (3.4)). For these devices and measurement conditions, $S_{vd}$ was observed to be of the “generic” $1/f^\alpha$ type. The extracted frequency exponent $\alpha$ varies between 0.7 and 1.1 for the devices of Fig. 6.4. The results in Fig. 6.4 (and those that follow) are representative of three nominally identical devices that showed similar results.

Fig. 6.3. Log-log plots of PSD of signal and background vs. frequency at 300 K with 0 V stress during heating. The signal noise is measured in the linear region of device operation, with $V_{DS} = -50$ mV and $V_{GS-V_{th}} = -0.6$ V. The background noise is measured with $V_{DS} = 0$ mV and $V_{GS-V_{th}} = -0.6$ V.
Fig. 6.4. Log-log plots of excess voltage noise power spectral density $S_{vd}$ vs. frequency in a temperature of 100 K to 440 K with 0 V stress during heating. The noise is measured in the linear region of device operation, with $V_{DS} = -50$ mV and $V_{GS} - V_{th} = -0.6$ V. The inset shows the threshold voltage as a function of temperature for fresh device. We measured the threshold voltage from $I_D - V_G$ curve at each temperature point to ensure that $V_{GS} - V_{th}$ was constant during the measurement of the temperature dependence of the $1/f$ noise.

Fig. 6.5 shows the excess drain voltage noise power spectral density (left hand scale) and frequency exponent $\alpha$ (right hand scale) for the unstressed device of Fig. 6.4. Both the noise magnitude $S_{vd}$ at 10 Hz and frequency dependence between 5 Hz and 40 Hz vary strongly with temperature. Excellent agreement is observed between the measured values of $\alpha$ (Eq. (3.5)) and predicted values obtained from Eq. (3.4) over the entire temperature region. For these calculations, the attempt time $\tau_0$ was estimated to be $1.8 \times 10^{-15}$ s, consistent with previous studies of MOS devices [49],[112],[113]. This confirms the applicability of the Dutta-Horn model of $1/f$ noise to these devices, and demonstrates that the noise is due to a random thermally activated process having a broad distribution of energies [48],[49],[53],[54]. This and studies of the temperature dependence of the noise in other MOS devices essentially rule out simple tunneling models, in which the rate-limiting steps in the $1/f$ noise of these MOS transistors were primarily
due to charge carriers tunneling into and out of traps in the oxide [49],[53],[114],[115]. The agreement between experimental data and the Dutta-Horn model allows us to estimate defect energy distributions $D(E_o)$ via Eq. (3.6), as we will discuss in Chapter 3.3.

Fig. 6.5. $S_{vd}$ at 10 Hz (left axis) and spectral slope $\alpha$ at 10 Hz as a function of temperature [right axis: red squares denote measured data, and blue circles denote calculated values from Dutta-Horn analysis via Eq. (3.4)].

6.2.2 Temperature dependence of 1/f noise with -2 V stress

Fig. 6.6 shows excess noise spectra $S_{vd}$ at different temperatures on the same device used in Fig. 6.4, but now with NBTS applied. The noise measurement conditions were similar to those of Fig. 6.4, except the device was stressed at a constant gate bias of -2 V for approximately 10 minutes between successive noise measurement as the device was heated from 100 K to 440 K. $I_D-V_G$ curves were measured before and 5 minutes after stress to allow recovery of the fast component of NBTI degradation before $V_{th}$ and 1/f noise measurements. A comparison of Figs. 6.4 and 6.6 shows that the threshold voltage of the device was modified by NBTS at higher
temperatures (insets), and the noise magnitude also significantly increases at higher temperatures. Fig. 6.1 above presents the comparative results of the noise measurements of Figs. 6.4 and 6.6, showing similar levels of noise at lower temperatures in stressed and unstressed devices, but significantly higher levels of noise for stressed devices at elevated temperatures. At ~ 430 K, for example, the noise of the stressed device is ~ 3× larger than that of the unstressed device. Because the noise of the unstressed device varies only weakly with temperature from ~ 260 K to ~ 430 K, we conclude that the increased noise in the stressed device results primarily from defects that are created by the NBTS.

Fig. 6.6. Log-log plots of excess voltage noise power spectral density $S_{vd}$ vs. frequency at four temperatures, for the device of Fig. 6.4, now subjected to NBTS. The noise is measured in the linear region of device operation, with $V_{DS} = -50$ mV and $V_{GS} - V_{th} = -0.6$ V. The inset shows the threshold voltage as a function of temperature for the stressed device. We measured the threshold voltage from an $I_D-V_G$ curve at each temperature point to ensure that $V_{GS} - V_{th}$ was constant during the measurement of the temperature dependence of the $1/f$ noise.
Fig. 6.7. Absolute values of threshold voltage shifts (left axis) and noise magnitude shifts at 10 Hz (right axis) versus temperature for stressed devices (Fig. 6.6), relative to the values for unstressed devices (Fig. 6.4). The solid curves are guides to the eye through the measured data.

Fig. 6.7 further compares the changes in noise and threshold voltage that are caused by NBTS in Figs. 6.1, 6.4, and 6.6. Here $\Delta S_{vd} = S_{vd,\text{stressed}} - S_{vd,\text{unstressed}}$, and $\Delta V_{th} = V_{th,\text{stressed}} - V_{th,\text{unstressed}}$. The magnitude of the change in threshold voltage with NBTS $\Delta V_{th}$ increases monotonically with increasing temperature, indicating an increase in the number of donor-like traps [42],[81],[106]-[110],[116]-[118]. The change in excess drain voltage noise power spectral density shift with NBTS $\Delta S_{vd}$ also tends to generally increase with temperature after NBTI stress. However, in contrast to the changes in $V_{th}$, the changes in $S_{vd}$ are not strictly monotonic. There are two possible reasons for this non-monotonicity in $\Delta S_{vd}$. The first is that, at least over a relatively small temperature range, some defects that lead to a significant amount of noise that are created at lower temperatures may anneal out thermally as the device is heated [49],[50],[106]-[108]. The second possibility is that defects are being created by NBTS that have a much more sharply peaked defect energy distribution than the defects introduced by device
processing [49],[50],[111],[112]. Each of these is quite plausible, as it is quite likely that both the defect density and energy distribution are changing as the device is subjected to NBTS [42],[106]-[108],[116]-[118], consistent with what happens when a device is exposed to ionizing radiation and then is annealed at elevated temperature [27],[49]-[51],[60],[111],[112],[119].

Fig. 6.8. Temperature dependent noise measurements at $f = 10$ Hz as a function of temperature ranging from 100 K to 440 K (bottom x-axis) before and after NBTI stress. The noise is measured under the same conditions as in Figs. 6.4 and 6.6. The temperature range corresponds to an energy barrier scale ranging from 0.26 eV to 1.13 eV (top x-axis). The concentration of defects increased significantly at energy barrier levels of ~ 0.77, ~ 0.95 and ~ 1.1 eV after the device was stressed at -2 V.

We now apply the Dutta-Horn model to estimate defect-energy distributions $D(E_o)$ in SiGe pMOSFETs with SiO$_2$/HfO$_2$ gate dielectric stack via Eq. (3.6). In Fig. 6.8, we plot $S_{vd}*f/T$ (proportional to $D(E_o)$) at $f = 10$ Hz as a function of temperature from 100 K to 440 K (bottom x-
axis) and energy $E_o$ via Eq. (3.7) from 0.26 eV to 1.13 eV (top x-axis). Before stress, the fresh device shows a large peak at low temperatures, and four smaller peaks in the defect-energy distribution at ~ 230 K (0.6 eV), ~ 260 K (0.65 eV), ~ 370 K (0.95 eV) and ~ 430 K (1.1 eV). The uncertainty in the inferred $E_o$ at each peak is ~ 0.025 eV due to the 10 K temperature increment. The stressed device shows all of these peaks and a new peak at ~ 300 K (0.75 eV). The magnitudes of the peaks at ~ 300 K, ~ 370 K, and ~ 430 K increase significantly with NBTS, while the lower energy peaks are affected less. The values of $E_o$ at higher energies (in the range 0.5–1.2 eV) inferred from the temperature dependence of the low-frequency 1/f noise of the stressed devices in Fig. 6.8 are quite consistent with the activation energies of individual defects in other devices with similar near-interfacial gate dielectric layers measured by other techniques, e.g., time dependent defect spectroscopy (TDDS) [117],[118].

### 6.2.3 Gate voltage dependence of low-frequency 1/f noise

As illustrated by the temperature dependence of the noise magnitude in Fig. 6.5, demonstrating the thermally activated nature of low-frequency noise, defects responsible for low-frequency noise in pMOSFETs are not usually distributed uniformly in energy and/or space. For thermally activated noise, it is not as easy to infer the spatial distribution of the defects, but varying the gate bias enables one to probe different regions of the Si/SiO$_2$ band gaps and provides useful and complementary information to varying the temperature [114]. If a peak exists in a non-uniform defect energy distribution, then varying the voltage also leads to a corresponding peak in noise vs. gate voltage, as following reasons: only traps near the Si/SiO$_2$ interface and within a few $kT$ of the quasi-fermi level communicate with the silicon; The fermi level changes with temperature while the trap energy levels move (relative to the fermi level) with gate voltage.
Fig. 6.9. Excess drain voltage noise power spectral density $S_{vd}$ at 10 Hz vs. $|V_{gs}-V_{th}|$ for SiGe pMOSFETs before and after NBTS at temperatures of (a) 210 K, (b) 300 K, (c) 370 K, and (d) 420 K. The noise is measured in the linear region of device response, with $V_{ds} = -0.05$ V and $|V_{gs}-V_{th}| = [0.2, 0.85]$ V. During NBTI, devices are stressed at $V_G = -2$ V for $10^4$ s, then annealed at 0 V gate bias stress for $10^4$ s to allow fast recovery of NBTI degradation as much as possible. Insets extract the slope of gate-source overdrive dependence of $S_{vd}$ at different temperatures.

Fig. 6.9 shows the pre- and post-stress excess drain voltage noise power spectral density $S_{vd}$ at 10 Hz and fixed $V_D = -50$ mV and extracted slope $\alpha$ over 5-40 Hz versus gate overdrive $V_{GS}-V_{th}$. The device with same geometries as one of Figs. 6.4 and 6.6 was stressed with $V_G = -2$ V (all other terminals were grounded during stressing) for during of $10^4$ s. Post-stress excess noise was measured after $10^4$ s recovery with $V_G = 0$ V after stress. Neither pre- nor post-stress $S_{vd}$ at 10 Hz shows clear peaks at the different temperatures which have been observed in temperature dependence of noise, suggesting that it is not easy to quantitatively map the voltage dependence of the noise into a defect-energy distribution. But the gate voltage dependence of noise can still provide us complementary information about defect distribution. Increase of noise magnitude after NBTI is observed at different temperatures except 210 K, indicating the defects associated with 300 K, 370 K and 420 K have major contribution to NBTI. This is consistent
with the results in Fig. 6.7. Only the slope at 300 K has an obvious change after NBTI, indicating the change of defect distribution caused by NBTI probably due to the reconfiguration after hole trapping. This is consistent with the results in Fig. 6.8. And $\alpha = \sim 1$ at 300 K (post-stress), 370 K (pre- and post-stress), 420 K (pre- and post-stress) is an evidence of uniform defect distribution, because generation of traps due to NBTS makes the trap density distribution more uniform. A $\alpha > 1$ (post-stress) at 210 K indicate there is an excess of slow sites which can be speeded up by raising the temperature [54]. Combining the temperature dependence and gate voltage dependence of low-frequency $1/f$ noise can identify the major defect energies contributing to NBTI: $\sim 0.77$ eV (configurational changes), $\sim 0.95$ eV and 1.08 eV. These defect states are essential for the understanding of the NBTI mechanism and modeling. The insets in Fig. 6.9 extract the slopes of drain voltage noise spectral density dependence on the gate voltage overdrive ($|V_{gs} - V_{th}|$) before and after NBTI stress. The slopes are strong temperature dependence and change greatly after NBTS because NBTS can change the non-uniform $D(E_o)$. At 300 K, the slope is -2.1 after NBTS, which highlights that the $1/f$ noise of SiGe devices is due to carrier number fluctuations [120]. This is not surprising since the SiGe channel can form an implant free quantum well (IFQW) which can significantly reduce the coulomb scattering from HfO$_2$/SiO$_2$ gate stack. At high temperatures, the slopes tend to be 1.0 after NBTS. The changes of slopes at different temperature after NBTS need further study.

6.3 Discussion

A significant number of experimental and theoretical studies have identified oxygen vacancy-related defects in SiO$_2$ as a dominant defect responsible for the low frequency $1/f$ noise of MOS transistors [27],[49]-[51],[60],[106]-[108],[119]. First-principles calculations based on density functional theory [121] have been used to identify oxygen vacancies in amorphous SiO$_2$
networks [112],[113]. At least two kinds of oxygen vacancies in amorphous SiO$_2$ are known to be important to this process. The first has a dimer configuration and is frequently identified with the $E'_\delta$-center [49],[112],[122]-[125]. The second is the $E'_\gamma$-center which has a dimer configuration in the neutral state and puckers in its positively charged state with significant lattice relaxation [22],[106],[112],[122]-[127].

For SiO$_2$, approximately 90% of oxygen vacancy defects exhibit little structural relaxation upon the capture of a hole, meaning that those defects still maintain the dimer configuration in the positively charged and neutral states [122]. The $E'_\delta$-center has been associated with shallow hole trapping and/or retarded hole transport in SiO$_2$ [122]-[125], with energies ranging from ~ 0.5 to ~1.0 eV [25],[112],[122]. So dimer O vacancies may contribute significantly to the noise observed between ~ 200 K and ~ 400 K in Fig. 6.8. Indeed, these defects may dominate the observed noise before and after stress at intermediate temperatures, e.g., the small peaks at energies of ~ 0.5 to ~ 0.65 eV in Fig. 6.8 that do not change with NBTS. Dimer O vacancies will not contribute to the relatively stable threshold voltage shifts observed at higher temperatures. But they are likely to contribute to the fast component of NBTI for measurements and above room temperature [22],[49],[106]-[108],[110],[117]. These defects do not undergo any permanent, structural changes through the NBTS process.

$E'_\gamma$-centers in SiO$_2$ have higher energies than $E'_\delta$-centers, and on the basis of a significant amount of work on MOS devices subjected to ionizing radiation and/or bias-temperature stress, are strong candidates for higher-energy noise peaks [36],[49],[50],[106]-[108],[116]-[118]. Complexes incorporating oxygen and hydrogen (e.g., the hydrogen bridge, which is a hydrogen atom at a dimer O vacancy in SiO$_2$ [37]-[39],[112],[128], and the hydroxyl $E'$ center, a strained O bonded to a hydrogen atom [40],[41]) may also affect the higher-temperature noise, especially
after NBTS. In contrast to the $E_{\delta}'$-centers, these defects are modified structurally and/or chemically via NBTS. Moreover, the hydrogen-related defects increase in density as a result of NBTS [37]-[41],[32],[91],[128].

Consistent with the above interpretation, we note that the regions throughout the interfacial layer SiO$_2$ and at the SiO$_2$/HfO$_2$ interface are rich in oxygen vacancies, as shown in Fig. 5.8. Moreover, calculations of oxygen-vacancy and/or hydrogen-related defect energy levels in HfO$_2$ show that similar defects in HfO$_2$ also likely contribute to the observed noise before and after NBTS [49],[70],[129]-[132]. The absence of the large peak at low temperatures in Fig. 6.8 in previous studies of the temperature dependence of the low-frequency noise of MOS transistors with SiO$_2$ gate dielectrics [49],[112],[113],[133] suggests that at least some of the low-energy peak in Fig. 6.8 may be associated with defects in the HfO$_2$ layer. However, we also note that the binding energy of atomic hydrogen at dopants in the SiGe layer drops to ~ 0.2 eV to ~ 0.3 eV under negative bias [134], suggesting that the capture and release of hydrogen by dopants in the SiGe channel layer may also contribute to the low-temperature noise peak in these devices. This process would occur on much faster time scales than can be sensed by low-frequency noise measurements at higher temperatures, where the noise appears to be dominant by the exchange of charge between the channel and the dielectric layers.

6.4 Summary and Conclusions of Chapter

We have measured the temperature dependence of the low-frequency $1/f$ noise of SiGe $p$MOSFETs with SiO$_2$/HfO$_2$ gate dielectrics with and without exposure to negative bias-temperature stress (NBTS). Information about defects contributing to NBTI is obtained for effective defect energy levels from ~ 0.2 eV to ~ 1.1 eV. At temperatures below ~ 270 K (energies below ~ 0.65 eV), the defects responsible for the low-frequency noise in these devices
are not significantly affected by NBTS. At higher temperature and energies, threshold voltage shifts due to NBTI are observed, as is a corresponding increase in noise. Noise at the lowest temperatures (< 200 K) may result primarily from defects in the HfO$_2$ layer and/or hydrogen motion in the SiGe layer. Noise at intermediate temperatures (200 K to 270 K) evidently results from dimer O vacancies in SiO$_2$. Noise at higher temperatures appears to result from a combination of hydrogen- and O-vacancy-related defects in the SiO$_2$ and/or HfO$_2$ layers. Noise levels in these particular devices at temperatures below ~ 270 K are not affected significantly by NBTS, but both levels at higher temperatures are affected quite significantly by NBTS. These results illustrate that both low-frequency noise and NBTI-related degradation in MOS transistors are affected strongly by several different types of defects that are distributed broadly in energy. Significant information about defect densities and effective energy distributions can be obtained via low-frequency noise measurements.
CHAPTER VII

Conclusions

This work has focused on the characterization of defects associated with TID and NBTI in the HfO$_2$/SiO$_2$ gate dielectric stack of pMOS transistors. In TID experiment, we find that negative bias irradiation leads to the worst-case degradation in the total dose response of SiGe pMOS FinFETs. We attribute this result to an increase in density of additional radiation-induced holes that become trapped in the HfO$_2$ under negative bias, and additional electron trapping under positive bias in the HfO$_2$, as compared with the 0 V irradiation case. A simple model of the structure suggests that these excess carriers originate in the near-interfacial SiO$_2$.

In the NBTI experiment, positive oxide-trap charge trapping is the dominant defect responsible for NBTI in Si$_{0.55}$Ge$_{0.45}$ pMOSFETs with high-K dielectrics. The experimental results show similarly small values of $E_a$ for oxide-trap charge buildup, while $E_a$ is lower for interface-trap buildup in the pMOSFETs with Si$_{0.55}$Ge$_{0.45}$ channel and high-K gate stacks, compared to the Si channel devices with SiO$_2$ gate dielectrics. The similar activation energies for oxide-trap charge in these two structures suggests that hole injection into the near-interfacial SiO$_2$ via tunneling is evidently the rate-limiting process for oxide-trap charge buildup during negative-bias stress. Electron energy loss spectroscopy shows the presence of Ge atoms in the Si capping layer. First-principles calculations show that Ge atoms near the Si/SiO$_2$ interface are primarily responsible for the reduced activation energies for interface traps in the SiGe pMOS devices, as compared with the Si pMOS devices.
The frequency and gate-voltage dependences of the low-frequency $1/f$ noise were investigated for SiGe $p$MOSFETs with SiO$_2$/HfO$_2$ gate dielectrics with and without exposure to negative bias-temperature stress (NBTS). Information about defects contributing to NBTI is obtained for effective defect energy levels from $\sim 0.2$ eV to $\sim 1.1$ eV. At temperatures below $\sim 270$ K (energies below $\sim 0.65$ eV), the defects responsible for the low-frequency noise in these devices are not significantly affected by NBTS. At higher temperature and energies, threshold voltage shifts due to NBTI are observed, as is a corresponding increase in noise. Noise at the lowest temperatures ($< 200$ K) may result primarily from defects in the HfO$_2$ layer and/or hydrogen motion in the SiGe layer. Noise at intermediate temperatures (200 K to 270 K) evidently results from dimer O vacancies in SiO$_2$. Noise at higher temperatures appears to result from a combination of hydrogen- and O-vacancy-related defects in the SiO$_2$ and/or HfO$_2$ layers. Noise levels in these particular devices at temperatures below $\sim 270$ K are not affected significantly by NBTS, but both levels at higher temperatures are affected quite significantly by NBTS. These results illustrate that both low-frequency noise and NBTI-related degradation in MOS transistors are affected strongly by several different types of defects that are distributed broadly in energy. Significant information about defect densities and effective energy distributions can be obtained via low-frequency noise measurements.
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