CHARACTERIZATION AND MODELING OF STRAINED SI FET AND GAN HEMT DEVICES

By

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A DISSERTATION PRESENTED TO THE GRADUATE SCHOOL OF THE UNIVERSITY OF FLORIDA IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE DEGREE OF DOCTOR OF PHILOSOPHY

UNIVERSITY OF FLORIDA

2011
To my family
ACKNOWLEDGMENTS

I sincerely thank my advisor, Prof. Scott E. Thompson, for his support, guidance, and giving me the opportunity of entering the challenge field of device characterization, analysis and design. I’d also like to thank my co-advisor, Prof. Toshikazu Nishida, for his guidance, encouragement and sharing of knowledge. Also, I thank my committee members, Prof. Jing Guo and Prof. Bhavani Sankar, for participating and evaluating my research work. And I thank Prof. Susan Sinnott for her instruction and discussion on the DFT topic.

I would like to especially thank all my colleagues: Amit, Andy, Guangyu, Hyunwoo, Jingjing, Ji-Song, Kehuey, Lu, Minki, Nidhi, Onur, Sagar, Sri, Tony, Toshi, Ukjin, Uma, Xiaodong, Yongke, Younsung, for their help and discussion during my graduate study.

Finally, I would like to show my greatest appreciation to my parents and my husband for their endless support.
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<td>Contact etch stop layers</td>
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<td>DOS</td>
<td>Density of states</td>
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<td>FNT</td>
<td>Fowler-Nordheim tunneling</td>
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<td>GGA</td>
<td>Generalized gradient approximation</td>
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<td>HEMT</td>
<td>High electron mobility transistor</td>
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<td>HSE</td>
<td>Heyd, Scuseria, and Ernzerhof</td>
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<td>LDA</td>
<td>Local density approximation</td>
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<td>MOSFET</td>
<td>Metal-oxide-semiconductor field-effect transistor</td>
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<td>PAW</td>
<td>Projector-Augmented Wave</td>
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<td>PBE</td>
<td>Perdew, Burke, and Ernzerhof</td>
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<td>PFE</td>
<td>Poole-Frenkel Emission</td>
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<td>SCE</td>
<td>Short channel effect</td>
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<td>SSOI</td>
<td>Strained silicon-on-insulator</td>
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<td>TFE</td>
<td>Thermionic field emission</td>
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<td>TG-FinFET</td>
<td>Tri-gate find-shaped field-effect transistor</td>
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<td>VLSI</td>
<td>Very large scale integrated</td>
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<td>2DEG</td>
<td>Two-dimensional electron gas</td>
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CHARACTERIZATION AND MODELING OF STRAINED SI FET AND GAN HEMT DEVICES

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December 2011

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Major: Electrical and Computer Engineering

Metal-oxide-semiconductor field-effect transistors (MOSFETs) have shown impressive performance improvements over the past 10 years by incorporating strained silicon (Si) technology. Concurrently, interest in alternate device structures and channel materials has been increasing tremendously because of the scaling limitations on performance enhancement. This work focuses on the impact of strain on state-of-the-art Si planar MOSFETs, Si tri-gate (TG) FinFETs, and GaN HEMT devices.

Piezoresistive properties of Si n- and pMOSFETs are obtained by applying controlled external mechanical stress, using the four-point and concentric-ring wafer bending setups. The results are discussed by considering strain-induced band splitting, band warping, and consequently the carrier repopulation, and the altered conductivity effective mass and scattering rate. Strain experimental results on TG FinFETs, coupled with the understanding of strained planar MOSFET physics, are used to explain the strain-enhanced tri-gate device performance.

Gallium Nitride (GaN) high electron mobility transistors (HEMTs) are promising for high-power applications, such as microwave or RF amplifiers. However the application
of these devices is limited by their reliability issues. A comprehensive study of the effects of mechanical stress on GaN HEMT channel resistance and gate leakage mechanisms is reported in this work. Using the tight binding method to calculate strained GaN band structure, the stress-altered channel resistance is simulated by considering two dimensional electron gas (2DEG) sheet carrier density and electron mobility variation. Several possible gate leakage mechanisms are modeled and compared to the experimental results. The Poole-Frenkel Emission from surface states is determined to be the dominant leakage mechanism and its stress dependence is investigated. Finally, the density functional theory (DFT) calculations based on various functionals are evaluated, and the HSE functional is employed to obtain the GaN band structure with correct bandgap.
CHAPTER 1
STRAIN ENGINEERING IN STATE-OF-THE-ART SI FET AND GAN HEMT

1.1 Motivation

In the past three decades, scaling of MOSFETs has resulted in new technology generations every two to three years with doubled logic device density, lowered cost per logic function, and increased chip performance [1-3]. However, as device dimension enters into the deep sub-micrometer regime, many physical phenomena such as short-channel effect (SCE), velocity saturation, high leakage current, and dielectric breakdown limit the benefits of conventional scaling [4-8]. To continuously improve device performance, new device structures, new materials, and strain engineering have been proposed and investigated. Among all these new technologies, strain engineering during the past decade has been the dominant technique to enhance device performance while providing a low-cost and low-risk technique by maintaining the traditional MOSFET fabrication process. With the fourth generation [9] of strained-Si technology now in commercial production, strain-enhanced performance and power saving are present in nearly all VLSI logic chips manufactured today.

As semiconductor device technology improves, strain is expected to be incorporated into new device structures and channel materials to provide potential improvement. To better predict the effect of strain in advanced technology, the strain-enhanced Si planar MOSFETs need to be characterized first, which serves as the foundation of understanding the role of strain in future technology.

Multi-gate devices, such as TG FinFETs, have the advantages of better electrostatic, large ON/OFF current ratio, and lower power. However, the multiple gates have different surface orientations that respond differently to stress. The overall performance enhancement is not straightforward and needs to be studied.

III-V materials have the potential to replace Si in the future, due to its higher electron mobility as well as wider choice of bandgap. Despite the GaN HEMT’s great potential for high power application, its performance is limited by reliability issues such as gate leakage current, hot electron injection, and barrier breakdown. Understanding the effect of stress on the failure mechanisms is crucial since additional strain occurs in HEMTs during device operation, due to the inverse piezoelectric effect.

1.2 Brief History of Strained Semiconductors

1.2.1 Strained Si FET

Strain has been a topic of interest in semiconductor research since the 1950s. Bardeen & Shockley [10] developed deformation potential theory, which models the coupling between acoustic waves and electrons in solids, to calculate the components of the relaxation-time tensor in terms of the effective mass, elastic constants, and a set of deformation-potential constants. In the deformation potential theory, the strain-induced band edge shift is proportional to the strain tensor,

$$\Delta E = \sum_{ij} \Xi_{ij} \varepsilon_{ij}$$  \hspace{1cm} (1-1)$$

where \( \Xi_{ij} \) are the deformation potentials. Herring & Vogt [11] generalized this theory in 1956 to model carrier transport in strained multi-valley semiconductors and summarized a set of independent deformation potentials, \( \Xi_d \), \( \Xi_u \), and \( \Xi_p \), to characterize the conduction band valleys. Their work ascribed the electron mobility change to “electron
transfer” and an altered intervalley scattering rate caused by the valley energy shift. The picture of strain-enhanced hole mobility is more complicated, owing to strong valence band warping. Thus, the hole transport under strain cannot be simply explained by band edge shift. Band structure calculations such as the $k \cdot p$ method [12-13] give more accurate valence band structure by constructing a strain Hamiltonian [14] in terms of the angular momentum derived by symmetry consideration. Hasegawa [15] and Hensel & Feher [16] used this method to systematically study the valence band effective masses and deformation potentials in strained Si. They revealed the key factors that affect the hole mobility in semiconductors—band splitting and warping, mass change, and consequently the change of DOS, which alters band occupation and phonon scattering. To date, deformation potential theory is still the primary method of modeling the strained semiconductor and has proven to be successful in explaining experimentally observed changes in device behavior under mechanical stress.

The most effective empirical method to predict device behavior under strain is by measuring the piezoresistance coefficients ($\pi$-coefficients) [17]. The first experimental data on $\pi$-coefficients for n- and p-type bulk Si and Ge were obtained by Smith in 1954 [18]. These data have been used by the industry to model and predict MOSFET current enhancement under stress. However, it is inappropriate to use them to analyze MOSFET behavior in some cases because Smith’s sample is bulk material without any surface confinement effect. In 1968, Colman et al. [19] measured the $\pi$-coefficients in p-type inversion layers for the first time. Two decades later, the first Si n- and pMOSFETs with biaxial stress induced by Si$_{1-x}$Ge$_x$ buffer layer (Figure 1-1A) were demonstrated by Wesler et al. [20] in 1992 and by Nayak et al. [21-22] in 1994,
respectively. A 2.2-times enhancement in electron mobility and a 1.5-times enhancement in hole mobility were reported. Rim et al. [23] investigated pMOSFETs drive current enhancement versus Ge content in Si$_{1-x}$Ge$_x$ layers in 1995 and measured the current enhancement for short-channel nMOSFETs in 1998 [24]. In 2005, Lee et al. [25] published a review of the history of and progress in high-mobility biaxially strained Si, SiGe, and Ge channel MOSFETs.

Figure 1-1. Illustration of process-induced stress on Si MOSFETs. A) Biaxial stress caused from lattice mismatch between the Si channel and the relaxed SiGe substrate. B) Uniaxial stress induced by the nitride capping layer.
Even though the predominant focus of the industry in the 1980s and 1990s was on biaxially stressed devices, the current focus has shifted to uniaxial stress. Uniaxial stress has several advantages over biaxial stress, such as larger mobility enhancements and smaller shift in threshold voltage [26]. Incorporating uniaxial stress to enhance MOSFET performance was first introduced by Ito et al. [27] and Shimizu et al. [28], who used etch-stop nitride (Figure 1-1B), and by Gannavaram et al. [29], who used SiGe source/drain (S/D) regions, in the early 2000s. Starting at the 90 nm technology node [30], uniaxial stress was successfully integrated into the mainstream MOSFET process flow to improve device performance [31-34]. Encouraged by the strain-enhanced planar MOSFETs, researchers recently applied uniaxial stress to multi-gate devices [35-40] with metal gate and high-k dielectric [41-42] as a performance booster. These studies demonstrate that strain achieves higher Si FETs performance with extensive industrial application.

1.2.2 Strained GaN HEMT

Unlike the strain technology in Si devices, stressing methods haven’t been intentionally used during device fabrication to alter GaN HEMT performance. Nevertheless, the AlGaN layer is under large biaxial tensile stress due to its lattice mismatch from the bottom relaxed-GaN substrate. In addition, since both the AlGaN and GaN are piezoelectric materials, the lattice deforms when an electric field is present. Under typical GaN HEMT operation conditions, the total stress in the AlGaN layer is approximately 3GPa or higher. This large amount of stress may vary the HEMT performance and reliability, and therefore has attracted researchers’ attention in the past one decade. Gaska et al. [43] applied biaxial compressive stress to study its effect on channel electron density. Their work observed decreasing electron density with
compressive stress. Eichhoff et al. [44], Kang et al. [45-46], Zimmermann et al. [47], Yilmazoglu et al. [48], and Koehler et al. [49] applied mechanical stress to investigate the piezoresistive property of GaN HEMTs. Large range of the extracted gauge factors was observed. Koehler et al. attributed this discrepancy to the charge trapping effects during electrical measurement. To investigate the effect of stress on HEMT reliability, del Alamo et al. [50-52] applied mechanical stress while electrically stressing the devices. They concluded that external tensile stress increases the gate leakage current and decreases the critical breakdown voltage. Using the mechanical bending stress as a tool, more thorough studies of the strained GaN HEMT performance and reliability are still going on to achieve better understanding.

In the future, the viability of novel structures and channel materials will depend on their ability to provide device enhancement comparable to strained-Si planar MOSFETs. Thus, strain will remain a necessary enhancement option even in these devices.

1.3 Objectives and Organization

In this work, the effects of strain on channel resistance and reliability of semiconductor devices with different structures and channel materials are investigated. Chapter 2 discusses the fundamental physics regarding the strained Si and GaN devices. In Chapter 3, a comprehensive set of two-dimensional (2D) inversion layer \( \pi \)-coefficients of Si planar MOSFETs is extracted and compared to the published surface \( \pi \)-coefficients as well as the corresponding bulk Si values. A qualitative argument for the reported differences due to quantum confinement is given. Based on the knowledge of planar MOSFETs, the measured longitudinal \( \pi \)-coefficients of long channel TG FinFETs are then discussed. Chapter 4 studies the strain-altered channel resistance of
AlGaN/GaN HEMT, in terms of 2DEG sheet carrier density and electron mobility. Strain is incorporated into a tight-binding model to simulate the gauge factor of HEMT devices, which will be compared to the experimentally extracted value to determine the best fit set of the elastic stiffness constants and piezoelectric coefficients of AlN and GaN. Chapter 5 addresses several possible gate leakage mechanisms in the GaN HEMT. The dominant mechanism is determined and its stress dependence is specified. The DFT strategy for GaN band structure and defect calculation is discussed in Chapter 6. Finally, a summary of this research is presented in Chapter 7.
CHAPTER 2
FUNDAMENTAL PHYSICS BEHIND STRAINED SI AND GaN DEVICES

Strain has been the main performance booster for Si MOSFETs in the past decade and has been intentionally incorporated into the device during fabrication. For the GaN HEMT, strain exists as an intrinsic device property due to lattice mismatch or arises from a non-zero gate electric field due to the inverse piezoelectric effect. To better model and explain the behavior of strained Si FET and GaN HEMT devices, the fundamental strain physics behind these devices operating under conventional conditions needs to be clarified. This chapter targets an overview of the strain and vertical electric field confinement effects on Si and GaN device performance, from the energy band structure perspective.

2.1 Strain and Stress

To obtain insights into the underlying physics of the strain-enhanced device, it is necessary to first understand strain, of which the effect on current drivability is usually quantified as a $\pi$-coefficient.

2.1.1 Strain Definition

Strain is defined as the percentage change of material’s lattice constant. Strain can result from lattice-mismatched film growth, phonon-induced lattice vibrations, and applied external mechanical stress. Beneficial strain reduces crystal symmetry, thus lifting band degeneracy and causing band warping. Any strain can be decomposed into a hydrostatic strain and two types of shear strain [53]. For cubic crystals such as Si and Ge, hydrostatic strain does not break crystal symmetry and, hence, only shifts energy
levels without lifting band degeneracy. Thus, it is not important for carrier mobility enhancement. Large hydrostatic strain is undesirable owing to band-gap narrowing, strain relaxation, and MOSFET threshold voltage shifts. It is the shear component of strain that causes subband splitting and affects semiconductor transport properties. Strain is introduced into the device channel preferably by applying uniaxial stress. The uniaxial stress is longitudinal when parallel to the channel and transverse when perpendicular to the channel.

Large magnitudes of uniaxial channel stress (\(\sim 1\ \text{GPa}\)) are being incorporated in p-channel devices of the 65-nm technology node [31-32], and an even higher stress level is applied in the 32-nm technology node, as is evident from the significantly large saturated drive current (1.55 mA/\(\mu\)m for NMOS and 1.21 mA/\(\mu\)m for pMOSFETs [9]). However, since many process-related parameters vary when fabricating strained MOSFETs, there is some uncertainty as to whether strain alone is responsible for the performance enhancement. To gain confidence in the effect of strain, external mechanical stress is applied using the four-point or concentric-ring wafer bending setup (Figure 2-1). In this work, the drive current enhancement under both uniaxial and biaxial stress is studied using these setups to predict the device performance of strained Si planar MOSFETs, TG FinFETs, and GaN HEMT devices.

2.1.2 Piezoresistance Coefficients

The \(\pi\)-coefficient gives straightforward experimental information about strain-enhanced carrier mobility in semiconductors. This coefficient is defined as the normalized change in resistivity per unit stress

\[
\pi = \frac{\Delta \rho}{\rho \cdot \sigma}
\]  

(2-1)
where $\sigma$ is the external stress and $\rho$ is the resistivity, which can be calculated by

$$\rho = \frac{1}{q\mu_n n + q\mu_p p}.$$  \hspace{1cm} (2-2)

For MOSFETs under steady state, the electron and hole densities are approximately constant, thus the $\pi$-coefficient is determined by the change in carrier mobility with stress. The $\pi$-coefficient gives us a straightforward idea about how much drive current enhancement can be achieved under particular stress, and therefore has been widely used in industry to predict strained device performance [54-56].

For cubic symmetric material such as Si, the longitudinal and transverse $\pi$-coefficients ($\pi_l$ and $\pi_t$) of any direction can be calculated from the piezoresistance tensor and direction cosines [57], and the biaxial $\pi$-coefficient ($\pi_B$) equals $\pi_l + \pi_t$. When a vertical electric field is applied (MOSFET cases), $\pi_l$, $\pi_t$, and $\pi_B$ may vary from their bulk value due to quantum confinement.

### 2.1.3 Wafer Bending

The standard four-point bending setup [58] is used to generate a uniaxial stress at the top surface of a rectangular wafer piece, as shown in Figure 2-1A. For Si samples, the surface stress $\sigma$ along the uniaxial stress direction (perpendicular to the rods) is calculated from the relation [59],

$$\sigma = \frac{EZt}{2a(\frac{L}{2} - \frac{2a}{3})}$$  \hspace{1cm} (2-3)

where $E$ is Young’s modulus of the stress direction, $Z$ is the sample vertical displacement, $t$ is the thickness of the sample, $a$ is the distance between the inner and outer rods, and $L$ is the distance between the two outer rods. This calculated uniaxial
stress showed good agreement with the independent measurement of a strain gauge mounted on the Si wafer surface (within 5% error to the actual stress measured by the resistance change in the strain gauge) as shown in Figure 2-2.

Figure 2-1. Illustrations of mechanically bended wafer samples. A) Four-point wafer bending for applying uniaxial stress. B) Concentric ring wafer bending for applying biaxial stress. © [2008] American Institute of Physics, [reprinted with permission from M. Chu et al., “Comparison between high-field piezoresistance coefficients of Si metal-oxide-semiconductor field-effect transistors and bulk Si under uniaxial and biaxial stress”, J. Appl. Phys., vol. 103, pp. 113704, Fig. 3 and Fig. 5, June 2008]

The rods are replaced by two concentric rings of different radii to generate a biaxial stress on a Si wafer piece, as shown in Figure 2-1B. Finite element method was
used to simulate the applied biaxial stress using ABAQUS, and two experimental methods (optical strain characterization from the measured wafer curvature and direct measurement using a strain gauge) were used to measure the induced biaxial stress versus the rings vertical displacement. The resulting stress calibration of the biaxial bending setup is shown in Figure 2-2. Good agreement is achieved between the Finite Element Analysis and the two independent measurements, and therefore this stress configuration will be used to calculate the biaxial $\pi$-coefficients.

Figure 2-2. Applied mechanical stress versus the vertical displacement of the top rods (uniaxial stress) or the top ring (biaxial stress) for Si MOSFET samples. Stress calibration is based on three different methods. © [2008] American Institute of Physics, reprint with permission from [M. Chu et al., “Comparison between high-field piezoresistance coefficients of Si metal-oxide-semiconductor field-effect transistors and bulk Si under uniaxial and biaxial stress”, J. Appl. Phys., vol.103, pp.113704, Fig. 4, June 2008]
For the GaN HEMT wafer samples, the strain gauge measurement is carried out to calibrate the 4-point wafer bending induced uniaxial stress and the result is shown in Figure 2-3.

![Graph showing strain gauge calibration of the applied uniaxial mechanical stress versus the graduation of stress for GaN HEMT samples.](image)

**Figure 2-3.** Strain gauge calibration of the applied uniaxial mechanical stress versus the graduation of stress for GaN HEMT samples.

### 2.2 Strained Si devices

Strain has a larger effect on the current conduction in Si than on a metal, owing to the fact that not only do the physical dimensions change under strain but the carrier mobility can also be enhanced. The effects of strain on carrier mobility in Si devices have been intensively studied over the past 10 years. Previous works [11, 60-62] pointed out that the main factors affecting mobility are (1) the change in the average effective mass due to carrier redistribution or band warping and (2) the change in the carrier scattering rate due to energy band splitting or density of state variation. Since
the applied vertical electric field in MOSFETs creates a potential well that confines the carrier in the transverse direction, the allowed energy levels are quantized. Therefore, in inversion-mode devices, the net energy band splitting is due to the cumulative effect of both strain-induced band splitting and 2D electrostatic surface confinement induced band splitting [60]. Furthermore, since confinement is a function of the transverse electric field caused by the applied gate voltage, in general, the surface $\pi$-coefficients may not be the same as the bulk Si $\pi$-coefficients.

2.2.1 Stress Effects on N-Si Band Structure

Figure 2-4. Schematic illustration of conduction band structure change under <110> uniaxial tensile stress for bulk n-type Si and Si (001)-nMOSFETs.
The Si conduction band minima are located near the X-point. Due to its crystal symmetry along the [100] major axis, there are six equivalent constant energy ellipsoids around each minimum. When external stress is present, the strain-induced conduction band edge shift is given by,

\[
\Delta E^i_c = \Xi_d \left[ Tr \left( \epsilon_{ij} \right) \right] + \Xi_a \left( k \epsilon_{ij} k \right)
\]

where \(\Xi_d\) and \(\Xi_a\) are the dilation and shear deformation potentials of the conduction band, respectively, \(i\) refers to one of the six valleys, \(Tr \left( \epsilon_{ij} \right)\) is the trace of the strain tensor \(\epsilon_{ij}\), and \(k\) is a unit vector in the reciprocal space [53]. The band edge shift can also be expressed in terms of hydrostatic band edge shift and shear band edge splitting by,

\[
\Delta E^i_c = \Delta E^i_{hydro} + \Delta E^i_{shear}
\]

where only the splitting term causes carrier redistribution and thus mobility change.

For example, the <110> longitudinal tensile stress causes the energy of the \(\Delta_2\) subband to shift down and the energy of the \(\Delta_4\) to shift up (the separation between \(\Delta_2\) and \(\Delta_4\) is calculated to be 40 meV under 1GPa using Eq. (2-4)), resulting in electrons repopulating from the \(\Delta_4\) valley to the \(\Delta_2\) valley, as shown in Figure 2-4. Because the conductivity effective mass of the \(\Delta_2\) valley (0.19\(m_0\)) is smaller than that of the \(\Delta_4\) valley (0.315\(m_0\), calculated using the method in [63]), the electron repopulation into the \(\Delta_2\) valley causes the average effective mass to decrease and carrier mobility to increase. The band splitting also alters the scattering rate. The dominant scattering mechanisms in strained n-Si devices are intervalley phonon scattering [64] and surface roughness scattering [65]. As the six-fold conduction bands split, the intervalley scattering rate
becomes lower owing to the smaller DOS [60], thus resulting in a higher mobility. A more complete discussion of phonon-limited electron mobility enhancement is provided by Takagi et al. [61].

Figure 2-5. Schematic illustration of valence band structure change under <110> uniaxial compressive stress for bulk p-type Si and Si (001)-pMOSFETs.

Strained nMOSFETs have different mobility enhancement factors from those of bulk Si. Because of the electric field confinement, the $\Delta_2$ and $\Delta_4$ valleys are originally non-degenerate for unstrained Si. The energy splitting between these valleys depends on the magnitude of the electric field and the difference in their out-of-plane confinement effective mass. It can be calculated from a self-consistent solution of the Schrödinger and Poisson equations [66]. Under low electric field, the band splitting without stress is
small, and thus the electron distribution does not differ much from the bulk Si. In contrast, as shown schematically in Figure 2-4, the band splitting without stress is already large under high electric field (>0.7 MV/cm), causing over 80% of electrons to be located in the low-energy valleys. Thus, further change in the average effective mass under stress is very small (<10%) [60]. Furthermore, surface roughness scattering dominates under typical commercial-use conditions for two-dimensional (2D) carrier transport, which makes the current transport in nMOSFETs more difficult to predictably model [67-68]. As a result, the high-field \( \pi \)-coefficients can differ significantly from the bulk \( \pi \)-coefficients but must converge to the bulk value as the transverse field goes to zero.

### 2.2.2 Stress Effects on P-Si Band Structure

The heavy-hole (HH) and light-hole (LH) valence band minima are degenerate at the \( \Gamma \)-point for bulk Si. In unstressed Si, 80% of the holes occupy the HH band, which has an effective mass of 0.59\( m_0 \) along the \(<110>\) direction (versus 0.15\( m_0 \) for the LH band). Compared to the n-Si band structure, the valence bands warp significantly under stress, which modifies the in-plane effective mass and the DOS [69]. Figure 2-5 schematically illustrates the valance band warping under \(<110>\) uniaxial compression. In the \(<110>\) direction, the HH band (top band) becomes LH-like around the \( \Gamma \)-point, and the LH band (bottom band) becomes HH-like. The top band is lower in energy and has smaller conductivity effective mass (0.11\( m_0 \) for 1GPa), whereas the bottom band is higher in energy and has larger conductivity effective mass (0.2\( m_0 \) for 1GPa). Most of the holes therefore repopulate into the top band, and the mobility is enhanced. As a result, not only the band edge but also the band structure close to the \( \Gamma \)-point is
important for hole transport, owing to the significant band warping. In addition, the HH, LH, and spin-orbit split-off hole bands are energetically close to each other, which makes the valence band structure calculation more complex. The valence band structure of bulk p-Si under stress can be numerically estimated, in particular, near the band edge using the k·p method with the Luttinger–Kohn strain Hamiltonian [13, 70]. At room temperature, band warping induced effective mass reduction is the dominant factor for mobility enhancement in p-type Si under uniaxial stress (<1GPa) [62]. The stress-induced phonon-scattering rate change is negligible [69], since the splitting between the top band and the bottom band is small compared with the Si optical phonon energy (61.3 meV).

For unstrained pMOSFETs, however, the degeneracy of the heavy hole and the light hole is lifted by the surface electric field confinement, as shown in Figure 2-5. Similar to the conduction band, the valence band structure can be calculated by solving the Schrödinger and Poisson equations self-consistently. Compared with the bulk Si energy contours, the transverse electric field splits the bands but does not modify the in-plane subband structure for the (001) surface devices, as shown in Figure 2-6 [69]. Therefore, the strain-induced hole effective mass change is expected to be similar for bulk p-Si and Si pMOSFETs. However, the in-plane DOS changes with stress (i.e., becomes smaller under uniaxial compression), which can cause a phonon scattering rate variation. We neglect this effect in bulk p-Si because the strain-induced band splitting (~20meV for 1GPa) is small compared to the optical phonon energy for Si. For the (001)-oriented pMOSFETs under typical operation condition (surface effective field $E_{eff}$~1MV/cm), the summation of confinement-induced band splitting and strain-induced
band splitting can be larger than the Si optical phonon energy, and the phonon scattering change cannot be neglected. As a result, the (001) pMOSFETs $\pi$-coefficients depend on both the DOS alteration and effective mass variation. For the (110)-oriented pMOSFETs, the electric field significantly modifies the in-plane band structure, as shown in Figure 2-7, which results in totally different mobility enhancement, and thus a variation of the 2D $\pi$-coefficients from the corresponding bulk values [69].

2.3 Strained GaN devices

Following the same process as strained-Si analysis, the band structure of wurtzite GaN is the starting point of investigating strain related GaN HEMT behavior. Nido [71] and Jogai [72] incorporated external stress into an empirical sp$^3$d$^5$ tight-binding model [73] to study the consequence of strain effects on the GaN band structure. Their work, however, considered only biaxial stress and focused mainly on the bandgap and valance band structure. Since the electron is the majority carrier in the GaN HEMT channel, it is essential to study the strain altered conduction band. In addition, uniaxial stress, which is the most beneficial stress for Si devices, is worth considering in GaN. Electron mobility altered by uniaxial stress is the main focus of this part of my research.

Similar to Si, electron mobility enhancement for bulk GaN can result from the average conductivity effective mass reduction and a suppression of intravalley scattering. Stress affects electron effective mass through two factors: band-splitting induced electron repopulation and band warping. Unlike Si which has six degenerate conduction bands, or GaAs which has energetically adjacent conduction bands, GaN is a direct band-gap material with only one conduction band, as shown in Figure 2-8. As a result, no electron repopulation occurs under stress, and thus band warping is the only
mechanism responsible for effective mass change. The absence of conduction band splitting also results in negligible change of the acoustic phonon scattering. The polar optical phonon scattering also has negligible dependence on stress, due to the fact that the mechanical stress does not induce polarization change along the longitudinal direction. Therefore, the change in effective mass through band warping is the dominant mechanism for stress-dependent bulk GaN electron mobility variation.

In a conventional GaN HEMT structure, a thin layer (10~30 nm) of AlGaN is deposited on top of a relatively thick layer (2~5 μm) of GaN, as shown in Figure 2-9. Due to the lattice mismatch between the AlGaN and GaN, the AlGaN layer is then considered biaxially stressed while the GaN layer is relaxed. Since both the AlGaN and GaN are piezoelectric materials, polarization appears in both layers. The total polarization difference between them gives rise to the 2DEG that forms on the GaN side of the interface between the AlGaN and GaN layers. For an Al fraction of 0.26, the 2DEG density is approximately $1 \times 10^{13}$ cm$^{-2}$. As a result, the channel forms even at zero gate bias and the GaN HEMT has negative threshold voltage. The 2DEG is confined at the interface and electron energy is quantized. However, there will not be confinement induced sub-band splitting in GaN HEMT since GaN has only one single conduction band. Therefore similar to bulk GaN, the scattering rate change in strained-GaN HEMT remains negligible and the band warping induced effective mass variation should dominate its stress behavior. The detailed modeling of strain-altered electron effective mass through conduction band warping will be discussed in Chapter 4.
Figure 2-6. The (001) 2D top-band energy contours (25, 50, 75, and 100 meV) with and without mechanical stress.  A) Bulk p-type Si.  B) The (001)-pMOSFETs.  
[Reprinted with permission from Sun G. 2007. PhD dissertation (Page.68-69, Figure 3-20 and 3-21). University of Florida, Gainesville, Florida].
Figure 2-7. The (110) 2D top-band energy contours (25, 50, 75, and 100 meV) with and without mechanical stress. A) Bulk p-type Si. B) The (110)-pMOSFETs. [Reprinted with permission from Sun G. 2007. PhD dissertation (Page.70-71, Figure 3-22 and 3-23). University of Florida, Gainesville, Florida].
Figure 2-8. Si and GaN subband E-k diagrams. A) For bulk Si [reprinted with permission from [74], Page 81]. B) For bulk GaN. Si has six degenerate conduction bands with minima locate near the X point. GaN has single conduction band locates at the \( \Gamma \) point.

Figure 2-9. A schematic of the conventional GaN HEMT structure. The band profile along the vertical direction (gate-AlGaN-GaN) is shown on the right side.
3.1 Introduction

Strained silicon is a preferred feature enhancement for high performance Si logic technology due to its advantage of enhancing channel carrier mobility and hence improving MOSFET performance [31, 34, 54, 75-76]. Since the 1990s, the physical understanding and modeling of carrier mobility enhancement due to strain has been aggressively studied for both n-type [60-61, 77] and p-type [60, 62, 65, 78-79] Si planar MOSFET inversion layers. The \( \pi \)-coefficient, which is defined as the normalized change in resistivity with applied stress, is one of the most useful parameters to capture and model the strain-altered current. The original \( \pi \)-coefficients for silicon and germanium were determined for bulk silicon and germanium by Smith [18] 50 years ago. Although the bulk Si \( \pi \)-coefficient values provide useful qualitative insight into the behavior of strained MOSFETs [54-56], it has been shown [19, 80-85] that 2D surface confinement effects caused by the vertical electric field, such as subband splitting and band warping, alter some of the \( \pi \)-coefficients. These works considered only uniaxial \( \pi \)-coefficients which were extracted under relatively low electric field (<0.7 MV/cm). It is only recently that the high-field \( \pi \)-coefficients (obtained from carrier mobility enhancement), under both uniaxial and biaxial stresses, were studied [86]. However, there is a need for a comprehensive comparison of confined \( \pi \)-coefficients under high
electric field for both n- and pMOSFETs under uniaxial and biaxial stresses for the (001) and (110) substrates, which is one of the focuses of this chapter.

Three-dimensional multi-gate (MG) transistors [87] such as tri-gate (TG) FinFETs [88] are potential alternatives to replace conventional MOSFETs at the 22nm node and beyond, because of their superior control of the Short Channel Effects (SCE) [87]. Meanwhile, strain has been widely used to enhance bulk Si MOSFET drive current [54]. These two technologies have been recently combined and additional performance enhancement in MG devices is achieved via process induced strain, such as $Si_xGe_{1-x}$, SiC in source/drain regions [36, 89-90], strained nitride contact etch stop layers (CESL) [91], supercritical strained-silicon-on-insulator (SC-SSOI) [37, 92-93], and strained SiGe-on-insulator (SSGOI) [35, 94]. However, since many process flow parameters are changed when incorporating strain, there is some uncertainty if strain alone is responsible for the performance enhancement. External mechanical stress applied by wafer bending is a direct method to study strain effect and reveal the underlining physics. Biaxial wafer bending on TG FinFETs was reported in [38], but few works investigate the effect of uniaxial stress, which is the proper stress for simultaneously improving n- and p-channel TG FinFET performance [40]. In this chapter, four-point wafer bending setup is used to apply uniaxial stress in the channel of TG FinFET. The longitudinal $\pi$-coefficients and their dependence on fin width and gate bias are extracted. A model is then proposed and validated to predict strained TG FinFET current enhancement.
3.2 Piezoresistance of Planar n- and pMOSFETS

3.2.1 Device and Experiment Details

In order to extract the 2D inversion layer $\pi$-coefficients, the strain-altered channel resistance was measured using n- and pMOSFETs on two surface orientations, (001) and (110) with two channel directions, namely (001)/<100>, (001)/<110>, (110)/<100>, and (110)/<110>. The details of the measured MOSFET devices are as follows: 10 $\mu$m/10 $\mu$m channel length/width, 1.2-1.4 nm gate oxide, n+/p+ polysilicon gates for n-/pMOSFETs, and $\sim 10^{18}$/cm$^3$ channel doping density. The channel resistances were measured by using a Keithley 4200 semiconductor parameter analyzer, under a gate effective field of $E_{\text{eff}} \sim 1$ MV/cm and a drain voltage of $|V_{ds}|=50$ mV.

There are two major sources of uncertainty during $\pi$-coefficient extraction: the uncertainty of applied stress and the uncertainty of device measurement. The total uncertainty of the extracted $\pi$-coefficients can be estimated by combining both factors.

$$U_\pi^2 = \left( \theta_{\Delta R/R} U_{\Delta R/R} \right)^2 + \left( \theta_\sigma U_\sigma \right)^2 \quad (3-1)$$

$$\theta_{\Delta R/R} = \frac{\partial \pi}{\partial (\Delta R/R)} = \frac{1}{\sigma} \quad (3-2)$$

$$\theta_\sigma = \frac{\partial \pi}{\partial \sigma} = -\frac{\Delta R/R}{\sigma^2} \quad (3-3)$$

where $U_{\Delta R/R}$ is the uncertainty of electrical measurement, $U_\sigma$ is the uncertainty of the applied stress, $\theta_{\Delta R/R}$ is the sensitivity coefficient of device measurement, and $\theta_\sigma$ is the sensitivity coefficient of the applied stress.

To calculate $U_\pi$, both $U_{\Delta R/R}$ and $U_\sigma$ must be investigated. In this study, $U_{\Delta R/R}$ is estimated as the 95% confidence interval of the $\Delta R/R$ measurements under stress. $U_\sigma$
is the uncertainty of each applied stress, which is estimated to be 1/5 of the minimum stress interval (4 MPa) used in this work. Using this process, the uncertainty estimates are listed in Table 3-1 for nMOSFETs and Table 3-2 for pMOSFETs, along with the corresponding extracted \( \pi \)-coefficients.

### 3.2.2 Results and Discussion

The stress-altered channel resistance \( \Delta R/R \) of the (001) surface \(<100>\) long-channel nMOSFETs is shown in Figure 3-1, including results under in-plane longitudinal, transverse uniaxial tensile stress, and biaxial tensile stress. Neglecting the geometrical contribution to \( \Delta R/R \), the \( \pi \)-coefficients are extracted by dividing \( \Delta R/R \) by the applied uniaxial stress calculated using Eq. (2-3), or biaxial stress which is experimentally determined using the calibration methods from Figure 2-2. Following the same process, the \( \pi \)-coefficients for both n- and pMOSFETs on the (001)/(110)-oriented surface with the \(<100>/<110>\) channel directions are extracted and summarized in Table 3-1 and Table 3-2, and compared with the bulk Si values from Smith.

#### 3.2.2.1 Stress results in n-type devices

Table 3-1 summarizes the extracted \( \pi \)-coefficients for nMOSFETs. The results show that the \( \pi \)-coefficients of (110)-oriented nMOSFETs are significantly different from the corresponding bulk value. For the (001)-oriented devices, however, the 2D \( \pi \)-coefficients are close to the bulk value for some particular cases.

The uniaxial \( \pi \)-coefficients show good agreement between the (001)/<110> nMOSFETs and Smith’s bulk value, while there is a large difference in the case of the (001)/<100> device (i.e. \( \pi_1=-102/-47, \pi_t=53/-22 \) for bulk Si and nMOSFETs, respectively). This difference is attributed to two factors: the high channel doping
density and the transverse electric field confinement. It is shown in [95] that the
electron mobility anisotropy decreases at high doping concentrations due to the
increased ionized impurity scattering. Therefore, the electron repopulation under stress
does not affect the average mobility as much as in the lowly doped sample. In addition,
most electrons are already located at the lowest energy valleys under electric field
confinement, which results in even lower strain-induced effective mass change. In this
case, variation of carrier scattering rate dominates the total mobility change. As a
result, the uniaxial \( \pi \)-coefficients of the (001)//<100> nMOSFETs can be significantly
smaller than the bulk value depending on its actual doping density and the applied gate
device. Figure 3-2 compares the extracted uniaxial \( \pi \)-coefficients of this work to the
literature. It confirms that the (001)//<110> nMOSFETs \( \pi \)-coefficients are relatively
insensitive to doping density and quantum confinement based on the similar
observations of many different devices. It also indicates a much wider variation for the
(001)//<100> device with higher doping density and effective field (~1 MV/cm). The \( \pi_l \)
and \( \pi_t \) can become smaller and, in fact, the \( \pi_l \) can change its sign under high effective
field if the scattering rate change is greater than the effective mass change.

For the (001)-oriented nMOSFETs under biaxial stress, the \( \pi \)-coefficient is not
much different from the bulk value, as shown in Table 3-1. This can be understood by
the fact that the electric field confinement effect on \( \pi_l \) and \( \pi_t \) cancel each other [82].
Since \( \pi_B = \pi_L + \pi_T \), the offset of confinement-altered \( \pi_L \) and \( \pi_T \) results in a \( \pi_B \) that is
almost independent of the vertical electric field. Figure 3-3 shows the measured (001)
\( \pi_B \) versus electric field, indicating little field dependence.
Figure 3-1. Strain-induced channel resistance change of the (001)/<100> nMOSFETs under longitudinal, transverse, and biaxial tensile stresses. The applied gate effective field is 1 MV/cm. © [2008] American Institute of Physics, reprinted with permission from [M. Chu et al., “Comparison between high-field piezoresistance coefficients of Si metal-oxide-semiconductor field-effect transistors and bulk Si under uniaxial and biaxial stress”, J. Appl. Phys., vol. 103, pp. 113704, Fig. 6, June 2008].

Table 3-1. Experimental extracted \( \pi \)-coefficients of Si planar nMOSFETs. They are compared to the corresponding bulk n-Si value from Smith. (Number in parentheses is the estimated uncertainty.) © [2008] American Institute of Physics, reprinted with permission from [M. Chu et al., “Comparison between high-field piezoresistance coefficients of Si metal-oxide-semiconductor field-effect transistors and bulk Si under uniaxial and biaxial stress”, J. Appl. Phys., vol. 103, pp. 113704, Table I, June 2008].

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<th>Surface Direction</th>
<th>Type</th>
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<th>( \pi_{2} )</th>
<th>( \pi_{3} )</th>
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<td>-22 (4.0)</td>
<td>-50 (2.3)</td>
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<td>53</td>
<td>-49</td>
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<td>-102</td>
<td>53</td>
<td>-49</td>
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<tr>
<td>(110) Channel</td>
<td>nMOSFETs</td>
<td>-37 (1.8)</td>
<td>11 (2.4)</td>
<td>-7 (3.9)</td>
</tr>
<tr>
<td>(110) Channel</td>
<td>Smith bulk</td>
<td>-31</td>
<td>53</td>
<td>-49</td>
</tr>
</tbody>
</table>
As a conclusion, the (001)-oriented nMOSFETs under biaxial stress have the largest $\pi$-coefficients which have little dependence on the vertical electric field. Results in Table 3-1 indicate that the surface-confined $\pi$-coefficients are not always the same as the bulk value, and Smith’s bulk data cannot be used to analyze highly doped (001)/<100> nMOSFETs operating under high vertical effective field.

![Figure 3-2. Extracted $\pi$-coefficients of this work compared to literature for the (001)-nMOSFETs. [18, 55, 80, 82, 84, 86, 96] The applied gate effective field is 1 MV/cm in our measurement. © [2008] American Institute of Physics, reprint with permission from [M.Chu et al., “Comparison between high-field piezoresistance coefficients of Si metal-oxide-semiconductor field-effect transistors and bulk Si under uniaxial and biaxial stress”, J. Appl. Phys., vol.103, pp.113704, Fig. 7, June 2008].](image-url)
Figure 3-3. Electric field dependence of biaxial $\pi$-coefficient for the (001)/<100> nMOSFETs. © [2008] American Institute of Physics, reprint with permission from [M. Chu et al., “Comparison between high-field piezoresistance coefficients of Si metal-oxide-semiconductor field-effect transistors and bulk Si under uniaxial and biaxial stress”, J. Appl. Phys., vol. 103, pp. 113704, Fig. 8, June 2008].

3.2.2.2 Stress results in p-type devices

Table 3-2 summarizes the extracted $\pi$-coefficients of Si pMOSFETs and the corresponding bulk value from Smith. The results show that the $\pi$-coefficients of (110)-oriented pMOSFETs are completely different from the corresponding bulk value. For the (001)-oriented devices, however, the 2D $\pi$-coefficients agree with the bulk value for most cases. Table 3-2 also lists the theoretical calculation results from [62], which have considered various surface/channel orientations, effective mass effect, phonon scattering effect, and surface roughness scattering effect. The theoretical results show good overall agreement with our experiment data, and thus confirm that the physical...
model of [62] can be used to explain the difference between pMOSFETs and bulk p-Si π-coefficients.

Table 3-2. Experimental extracted π-coefficients of Si planar pMOSFETs. They are compared to the corresponding bulk p-Si value from Smith and the simulated value from [62]. (Number in parentheses is estimated uncertainty.) © [2008] American Institute of Physics, reprint with permission from [M.Chu et al., “Comparison between high-field piezoresistance coefficients of Si metal-oxide-semiconductor field-effect transistors and bulk Si under uniaxial and biaxial stress”, J. Appl. Phys., vol.103, pp.113704, Table II, June 2008].

<table>
<thead>
<tr>
<th>Surface/Channel</th>
<th>p-MOSFET</th>
<th>πl</th>
<th>πt</th>
<th>πB</th>
</tr>
</thead>
<tbody>
<tr>
<td>(001) Surface</td>
<td>p-MOSFET</td>
<td>-15 (6.4)</td>
<td>9 (4.3)</td>
<td>11 (3.7)</td>
</tr>
<tr>
<td>&lt;100&gt; Channel</td>
<td>Smith bulk Si</td>
<td>6.6</td>
<td>-1.1</td>
<td>5.5</td>
</tr>
<tr>
<td>(001) Surface</td>
<td>p-MOSFET</td>
<td>71 (15.6)</td>
<td>-32 (7.7)</td>
<td>16 (5.8)</td>
</tr>
<tr>
<td>&lt;110&gt; Channel</td>
<td>Smith bulk Si</td>
<td>72.7 [62]</td>
<td>-45.8 [62]</td>
<td>5.5</td>
</tr>
<tr>
<td>(110) Surface</td>
<td>p-MOSFET</td>
<td>31.3 (1.0)</td>
<td>-9.5 (1.0)</td>
<td>25.4 (2.4)</td>
</tr>
<tr>
<td>&lt;100&gt; Channel</td>
<td>Smith bulk Si</td>
<td>6.6</td>
<td>-1.1</td>
<td>5.5</td>
</tr>
<tr>
<td>(110) Surface</td>
<td>p-MOSFET</td>
<td>27 (8.8)</td>
<td>-5 (3.0)</td>
<td>25.8 (2.2)</td>
</tr>
</tbody>
</table>

Our results show that the (001)/<110> pMOSFETs have the largest π-coefficients, followed by the (110)-substrate devices, and then the (001)/<100> devices. The π-coefficients for the (001)-oriented pMOSFETs, except the (001)/<110> transverse result, agree with the bulk value and have little vertical electric field dependence [86]. This can be understood from the complementary effects of DOS alteration on reducing the scattering and reducing the effective mass for these stresses [62]. For the (001)/<110> pMOSFETs under transverse stress, in contrast, these two effects are subtractive (i.e., increased effective mass with decreased scattering under transverse compressive stress), which results in a smaller mobility change than bulk p-Si. As a result, the corresponding π-coefficient is smaller than the bulk value. Detailed discussion of the strain-induced change in the hole mobility can be found in [62].
general, while the strain-induced band warping, band splitting, and 2D DOS alteration alter the effective mass and scattering rate, the confinement induced band splitting also affects carrier distribution and scattering. Both of these effects must be included to investigate the strain effect on pMOSFETs.

Figure 3-4. Extracted $\pi$-coefficients of this work compared to literature for the (001)-pMOSFETs. [18-19, 55, 80, 82, 84, 86, 96] The applied gate effective field is 1 MV/cm in our measurement. © [2008] American Institute of Physics, reprint with permission from [M.Chu et al., “Comparison between high-field piezoresistance coefficients of Si metal-oxide-semiconductor field-effect transistors and bulk Si under uniaxial and biaxial stress”, J. Appl. Phys., vol.103, pp.113704, Fig. 9, June 2008].

Figure 3-4 compares the extracted pMOSFETs uniaxial $\pi$-coefficients of this work to the literature which shows good overall agreement. For pMOSFETs under a
relatively low biaxial stress (<200 MPa), the $\pi$-coefficients are much smaller than the (001)/<110> uniaxial value, because of the smaller effective mass change under biaxial stress than uniaxial stress [69]. Therefore, only small current enhancement is expected for biaxial-stressed devices and uniaxial stress is more advantageous for pMOSFETs.

In summary, our result in Table 3-2 shows that the (001)/<110> pMOSFETs under longitudinal stress have the largest $\pi$-coefficients with little vertical electric field dependence, and Smith’s bulk value can be used to analyze the (001)-oriented pMOSFETs, except for the (001)/<110> transverse stress. For devices on the (110) substrate, surface confinement must be taken into account.

3.3 Piezoresistance of TG FinFETs

3.3.1 Device and Experiment Details

The TG FinFETs were fabricated on (001)-oriented SOI wafers with 145nm buried oxide (BOX) and 65nm starting silicon layer [37]. Fins with widths varying from 10um down to 20nm were patterned using 193nm lithography. The fins were left un-doped. The gate stack consists of a 2nm thick HfO$_2$ dielectric deposited by atomic-layer-chemical-vapor-deposition (ALCVD) and a 5nm TiN layer that is capped with 100nm polysilicon. NiSi was used as a salicide. Figure 3-5A shows the TEM image of the finished device. The fin length $L$, width $W$, and fin height $H$ are defined as shown schematically in Figure 3-5B. All devices have <110> channel direction and (110) side wall. Uniaxial stress was applied via 4-point wafer bending [83] for 10um long TG FinFETs with varying fin widths and the $\pi$-coefficients were extracted under a gate over-drive ($V_G-V_{TH}$) ranging from 0.2V~0.7V.
3.3.2 Experimental Results

In this section, experimental results of the extracted \( \pi \)-coefficients for both n- and p-channel TG FinFETs are reported. Figure 3-6 and Figure 3-7 show the \( \pi \)-coefficient dependence on the fin width of n- and p-channel TG FinFETs, respectively. With decreasing fin width, it is observed that the \( \pi \)-coefficients increase slightly from -29 to -38 for n-channel devices, whereas they decrease dramatically from 53 to 25 for p-channel devices. Table 3-3 summarizes the \( \pi \)-coefficients for TG FinFETs with \( W=10\mu m \) and \( 0.02\mu m \), along with the (001) and (110) planar MOSFETs values [17], as well as the results reported in [39] for DG FinFETs.

![Illustrations of the TG FinFET structure. A) TEM image of a 20nm wide Fin. B) Schematic structure of a Fin with \( W=H \). C) Schematic structure of a Fin with \( W>>H \). D) Schematic structure of a Fin with \( W<<H \).](image)

Figure 3-5.
Figure 3-6. The dependence of n-channel TG FinFET $\pi$-coefficients on the fin width. The solid curve is the theoretical value calculated by weighted averaging (001) and (110) surface $\pi$-coefficients with respect to fin width and fin height.

Table 3-3. The longitudinal $\pi$-coefficients ($\times 10^{12}$ dyne/cm$^2$) for n- and p-channel TG FinFETs. Our extracted results are compared to the literature published values for the (001), (110) planar MOSFETs and DG FinFETs.

<table>
<thead>
<tr>
<th>Device Type</th>
<th>P-channel</th>
<th>N-channel</th>
</tr>
</thead>
<tbody>
<tr>
<td>TG FinFET (W = 10 um)</td>
<td>53</td>
<td>-29</td>
</tr>
<tr>
<td>TG FinFET (W = 0.02 um)</td>
<td>25</td>
<td>-38</td>
</tr>
<tr>
<td>Planar MOSFETs [17]</td>
<td>(001) surface: 71.8</td>
<td>(001) surface: -31.5</td>
</tr>
<tr>
<td></td>
<td>(110) surface: 27.3</td>
<td>(110) surface: -37.0</td>
</tr>
<tr>
<td>DG FinFETs [39]</td>
<td>37</td>
<td>-51.4</td>
</tr>
</tbody>
</table>

The $\pi$-coefficient of n-channel TG FinFETs with W=10um (-29) is close to the (001) planar nMOSFETs value (-31.5 [17]). For n-channel device with W=0.02um, the $\pi$-coefficient (-38) is the same as the (110) planar nMOSFETs value (-37 [17]), but
smaller than the DG n-FinFET value (-51.4 [39]). The $\pi$-coefficient of p-channel TG FinFETs with $W=10\mu m$ (53), however, is smaller than the (001) planar pMOSFETs value (71.8 [17]). For p-channel TG device with $W=0.02\mu m$, the $\pi$-coefficient (25) is similar to the (110) planar pMOSFETs value (27.3 [17]) but smaller than the DG p-FinFET value (37 [39]).

Figure 3-7. The dependence of p-channel TG FinFET $\pi$-coefficients on the fin width. The solid curve is the theoretical value calculated by weighted averaging (001) and (110) surface $\pi$-coefficients with respect to fin width and fin height.

The TG FinFETs $\pi$-coefficient dependence on the gate overdrive voltage is also extracted, and the results for n- and p-channel devices are plotted in Figure 3-8 and Figure 3-9, respectively. Figure 3-8 shows that the gate bias has negligible effect on
the $\pi$-coefficient for both wide and narrow n-channel TG FinFET. The variation is less than 5%. For p-channel TG FinFET $\pi$-coefficient as shown in Figure 3-9, however, strong dependence on gate bias is observed in wide-width devices, whereas no evidence of gate bias dependence is seen in narrow-width device.

![Piezoresponse Coefficients](image)

**Figure 3-8.** Experimentally observed dependence of the $\pi$-coefficients on gate overdrive for n-channel TG FinFET.

### 3.3.3 Discussion

By investigating the $\pi$-coefficient dependence on the fin width and the gate overdrive voltage, the strain-enhanced TG FinFET behavior can be explained and predicted. The experimental results are compared to the theoretical expectation, and the discrepancy is discussed in this section.
Figure 3-9. Experimentally observed dependence of the \( \pi \)-coefficients on gate overdrive for p-channel TG FinFET.

3.3.3.1 A model for strain-enhanced TG FinFETs

The experimental results can be explained by a theoretical model which weighted averages the (001) and (110)-surface \( \pi \)-coefficients, as shown in Eq. 3-4.

\[
\pi_{\text{ave}} = \frac{\pi_{001} \cdot W + \pi_{110} \cdot 2H}{W + 2H}
\]  

(3-4)

From this model, when \( W \gg H \) (Figure 3-5C), current conduction on the top surface dominates and the stressed TG FinFET behavior is expected to be the same as a (001)-surface strained planar MOSFET. In contrast, when \( W \ll H \) (Figure 3-5D), it is expected that the strained TG FinFET behavior is the same as a (110)-surface strained planar
MOSFET because the (110) side wall conduction dominates. For very thin $W$ ($W<20\text{nm}$), bulk inversion become significant [97-98] and the TG FinFET should show similar strain-induced enhancement as a DG FinFET.

3.3.3.2 N-channel TG FinFET behavior

Over the entire fin width range down to 20nm, the experimental extracted $\pi$-coefficients agree with the theoretical model, as shown in Figure 3-6. Furthermore, the TG FinFET $\pi$-coefficients have negligible dependence on gate overdrive, which is also similar to the $\pi$-coefficients of strained planar n-channel MOSFETs with $<110>$ channel. This is because the $\Delta_2$ subband warping under $<110>$ uniaxial stress does not depend on the confinement-induced splitting [60]. As a result, for n-channel TG FinFETs down to 20nm in width, strained current enhancement can be modeled by the (001) and (110) planar MOSFET $\pi$-coefficients, with no observation of higher $\pi$-coefficient value caused by bulk inversion as in DG FinFET.

3.3.3.3 P-channel TG FinFET behavior

The extracted $\pi$-coefficients match the theoretical model for narrow-width TG FinFETs where side wall conduction dominates. However, the data for wide-width TG FinFET is smaller than the theoretical value. This discrepancy can be understood by the gate overdrive dependence of the TG FinFET $\pi$-coefficient, as plotted in Figure 3-9. The figure shows a decreasing $\pi$-coefficient versus increasing gate overdrive for large-width devices and a constant $\pi$-coefficient for devices with small fin width. Because of the un-doped fin body and the small electric oxide thickness, inversion carrier density increases rapidly under gate bias and can reach a level over $1.5 \times 10^{13} /\text{cm}^2$. The simulation done in [69] indicates that the $\pi$-coefficient for (001) planar MOSFETs
becomes less than 2/3 of its original value at this density level and beyond, which matches our result for large-width TG FinFETs. For small fin width, however, the $\pi$-coefficient keeps relatively constant even with high carrier density. This is because the subband splitting between the top two valence bands for (110) surface is so large (>60 meV [62]) that the variation of splitting caused by changing the gate overdrive does not affect the carrier distribution.

As discussed above, the current enhancement of strained p-channel TG FinFETs strongly depends on the gate bias if the fin width is large. For narrow-width device, its strain-enhanced performance can be modeled by (110) planar MOSFETs $\pi$-coefficient and there is no observation of higher $\pi$-coefficient value caused by bulk inversion as in DG FinFETs.

### 3.4 Conclusion

Piezoresistance coefficients of MOSFETs with different surface orientations and channel directions are measured under longitudinal, transverse, and biaxial stresses. The results are compared to the bulk Si value from Smith and to other literature publications. The extracted $\pi$-coefficients of the (110) MOSFETs are significantly different from the bulk value, and the surface confinement effect must be taken into account. For the (001) nMOSFETs, the uniaxial $\pi$-coefficients strongly depend on the doping density, electric field, and channel direction. The magnitude of the (001) $\pi_B$ is comparable to that of $\pi_l$ and is insensitive to the vertical electric field, making biaxial stress promising for nMOSFETs. For the (001) pMOSFETs, the (110) longitudinal uniaxial stress has the highest $\pi$-coefficient which has little dependence on the vertical electric field, and therefore is the most advantageous stress for pMOSFETs.
The longitudinal $\pi$-coefficients of n- and p-channel TG FinFETs with fin width down to 20nm were measured and compared to the planar MOSFET and DG FinFET values. Within the entire fin width range, the strain induced current enhancement for n-channel TG FinFET can be modeled by a linear combination between the (001) and (110) planar $\pi$-coefficients. For p-channel TG FinFET, the $\pi$-coefficient of narrow-width device matches the theoretical prediction, whereas the $\pi$-coefficient for wide fins is smaller than the (001) planar MOSFET value due to a high carrier concentration in the undoped channel. Both experiment and theoretical results prove that longitudinal stress is beneficial for TG FinFET current transport.
CHAPTER 4
EFFECT OF STRESS ON GAN HEMT RESISTANCE

4.1 Introduction

AlGaN/GaN high-electron-mobility transistors (HEMT) have great potential for high voltage switching and broad band power applications [90-91], owing to the large band gap of GaN [99]. Despite the HEMT device’s promising performance, its reliability can be impaired by the inverse-piezoelectric effect [50-52], which generates unexpected mechanical stress while the device is operated under high voltage. To clarify the stress effect on HEMT reliability, the stress-altered channel resistance has been studied, which is a good indicator on reliability issues such as hot electron injection [100].

Gauge factors have been extracted experimentally in previous works [43-48], though the results were confusing due to their large variation from -4 to -40,000. Koehler et al. [49] recently reported a gauge factor of -2.4±0.5 and attributed the large variation in literature to the existence of trapping effects during measurement. To better understand the stress effect on HEMT device channel resistance and determine a reasonable gauge factor, a simulation model is developed in this chapter by considering the stress-altered two-dimensional electron gas (2DEG) sheet carrier density and electron mobility. For the first time, uniaxial stress is incorporated into an sp^3d^5 empirical tight-binding model to investigate the stress effect on electron effective mass in wurtzite GaN.

4.2 Theory and Modeling

The channel resistance of the AlGaN/GaN HEMT device is inversely proportional to the 2DEG sheet carrier density ($n_s$) and channel electron mobility ($\mu_e$). This section
describes the model and procedure that are used to study the stress effect on \( n_S \) and \( \mu_e \). Simulation uncertainty is investigated to ensure more accurate results.

4.2.1 Stress Dependence of 2DEG Sheet Carrier Density

The 2DEG forms at the interface of the AlGaN and GaN layers, arising from the total polarization difference between them [101]. There are two types of polarization: spontaneous polarization \( (P^{SP}) \) and piezoelectric polarization \( (P^{PE}) \). Spontaneous polarization exists in both AlGaN and GaN layers, since their \( \sqrt{c/a} \) ratio differs from the ideal wurtzite crystal value \( (\sqrt{8/3}) \). Piezoelectric polarization arises from the piezoelectric effect, which is proportional to the strain. In the “as-fabricated” AlGaN/GaN HEMT structure, a thin layer of strained AlGaN due to lattice mismatch is on top of a thick layer of relaxed GaN. As a result, piezoelectric polarization exists only in the AlGaN layer without external stress. Figure 4-1A schematically shows the total polarizations in the “as-fabricated” device. From the total polarization difference between the AlGaN and GaN layers, \( \sigma = P(AlGaN) - P(GaN) \), the 2DEG sheet carrier density can be calculated using Eq. (4-1) [101],

\[
n_S(x) = \frac{+\sigma(x)}{q} \left[ \varepsilon_0 \varepsilon(x) \left( \frac{\varepsilon(x)}{dq^2} \right) \right] \left[ q \phi_b(x) + E_F(x) - \Delta E_C(x) \right]
\]

where \( x \) is the Al content, \( \sigma \) is the total polarization difference between AlGaN and GaN layers, \( \varepsilon \) is the dielectric constant, \( d \) is the depth of the AlGaN layer, \( q \phi_b \) is the Schottky-Barrier of a gate contact, \( E_F \) is the Fermi level with respect to the GaN conduction-band-edge energy, and \( \Delta E_C \) is the conduction band offset at the AlGaN/GaN interface. This work uses an Al-content of 0.26.
External mechanical stress affects the 2DEG density by generating additional piezoelectric polarization along the [0001] direction. Spontaneous polarization stays the same since it is an intrinsic material quality. When external stress is applied, additional piezoelectric polarization arises in both layers as shown in Figure 4-1B. The amount is proportional to the strain and piezoelectric coefficients ($P_{PE,mach}^{PE} = e_{ij} \cdot \varepsilon_{ij}$). In this work, the AlGaN and GaN layers are assumed to have the same level of strain, due to the fact...
that in most mechanical-bending experiment both layers of the AlGaN/GaN HEMT are significantly thinner than the substrate and therefore are located near the top surface of the wafer. In addition, the piezoelectric coefficients of AlGaN and GaN are similar. As a result, the difference between the strain-induced piezoelectric polarizations of these two layers is close to zero. Therefore, we expect that external stress has little effect on the 2DEG sheet carrier density.

4.2.2 Stress Dependence of Channel Electron Mobility

It has been concluded in Chapter 2 that the mechanical stress alters the channel electron mobility mainly through band warping induced effective mass change. We use an sp$^3$d$^5$ empirical tight-binding method developed in [73] to calculate the GaN band structure and electron effective mass. The unit cell of wurtzite GaN contains four atoms, two anions (N) and two cations (Ga) as shown in Figure 4-2A. All nearest-neighbor s, p, and d interactions, as well as second-nearest-neighbor s and p interactions are included using two-center approximation [102], which results in a 26×26 Hamiltonian matrix. The tight-binding parameters used in this work, including five on-site one-center, eight nearest-neighbor two-center, and eight second-nearest-neighbor two-center integrals, are listed in Table IV of [73]. The GaN band structure is obtained by solving the eigenvalue of the Hamiltonian matrix. The electron effective mass is then calculated along the $\Gamma$-M, $\Gamma$-K, and $\Gamma$-A directions in the reciprocal lattice as shown in Figure 4-2B.

The effect of mechanical stress is incorporated into the tight-binding model by considering the strain-induced change in atom location, which results in varied bond
length, bond angle, and reciprocal lattice. In this work, in-plane biaxial stress and uniaxial stress along the x and y axis as shown in Figure 4-2A are considered.

Figure 4-2. Wurtzite GaN structures in the real and reciprocal spaces. A) Unit cell with 4 basis atoms, where 1 and 3 are Ga atoms, 2 and 4 are N atoms. B) The reciprocal lattice for unstrained wurtzite GaN. Electron effective mass is calculated along $\Gamma$-K, $\Gamma$-M and $\Gamma$-A directions. © [2010] American Institute of Physics, reprint with permission from [M. Chu et al., “Simulation of AlGaN/GaN high-electron-mobility transistor gauge factor based on two-dimensional electron gas density and electron mobility”, J. Appl. Phys., vol.108, pp.104502, Fig.5, November 2010].

Under biaxial stress, the hexagon in the c-plane does not deform but only varies in size as shown in Figure 4-3A. The resulting strain in all three directions is related to the applied stress through Eq. (4-2) and (4-3),

$$\varepsilon_{xx} = \varepsilon_{yy} = \frac{C_{33}}{(C_{11} + C_{12})C_{33} - 2C_{13}^2} \cdot \sigma$$  \hspace{1cm} (4-2)

$$\varepsilon_{zz} = \frac{-2C_{13}}{(C_{11} + C_{12})C_{33} - 2C_{13}^2} \cdot \sigma$$  \hspace{1cm} (4-3)
where $\sigma$ is the biaxial stress, and $C_{11}$, $C_{12}$, $C_{13}$, and $C_{33}$ refer to the GaN elastic stiffness constants. The primitive translation vectors in rectangular coordinates becomes

$a_1 = [a(1 + \varepsilon_{xx}), 0, 0], a_2 = [-a/2(1 + \varepsilon_{xx}), \sqrt{3}a/2(1 + \varepsilon_{yy}), 0], \text{ and } a_3 = [0, 0, c(1 + \varepsilon_{zz})]$,

where $a$ is the length of a hexagon side and $c$ is the repeat distance in the $z$ direction.

The corresponding reciprocal lattice vectors are $b_1 = [2\pi/(a(1 + \varepsilon_{xx})), 2\pi/(\sqrt{3}a(1 + \varepsilon_{yy})), 0], b_2 = [0, 4\pi/(\sqrt{3}a(1 + \varepsilon_{yy})), 0], \text{ and } b_3 = [0, 2\pi/(c(1 + \varepsilon_{zz}))]$. The reciprocal lattice, under biaxial stress, remains a hexagonal shape. The basis vectors, where the atoms are located, are $t_1 = [0, \sqrt{3}a/3(1 + \varepsilon_{yy}), 7c/8(1 + \varepsilon_{zz})], t_2 = [0, 0, 0], t_3 = [0, 0, 3c/8(1 + \varepsilon_{zz})], \text{ and } t_4 = [0, \sqrt{3}a/3(1 + \varepsilon_{yy}), c/2(1 + \varepsilon_{zz})]$. The strain-varied bond length and bond angle between all nearest and second-nearest-neighbors can then be calculated based on the new atom locations. Since the atomic layout in the $c$-plane remains hexagonal, the expressions of elements in the $26 \times 26$ Hamiltonian matrix do not change. The stress-dependent band structure calculation is straight forward, with the bond length and bond angle the only parameters needed to be changed.

Under uniaxial stress, however, the in-plane hexagonal shape is deformed as shown in Figure 4-3B. The resulting strain in all three directions is related to the applied stress through Eq. (4-4), (4-5) and (4-6).

$$\varepsilon_{xx} = \frac{C_{11}C_{33} - C_{13}^2}{C_{11}(C_{11}C_{33} - 2C_{13}^2) - C_{12}(C_{12}C_{33} - 2C_{13}^2)} \cdot \sigma$$  \hspace{1cm} (4-4)

$$\varepsilon_{yy} = \frac{-\left(C_{12}C_{33} - C_{13}^2\right)}{C_{11}(C_{11}C_{33} - 2C_{13}^2) - C_{12}(C_{12}C_{33} - 2C_{13}^2)} \cdot \sigma$$  \hspace{1cm} (4-5)

$$\varepsilon_{zz} = \frac{C_{13}(C_{12} - C_{11})}{C_{11}(C_{11}C_{33} - 2C_{13}^2) - C_{12}(C_{12}C_{33} - 2C_{13}^2)} \cdot \sigma$$  \hspace{1cm} (4-6)
Figure 4-3. Lattice projection on the c-plane of GaN under externally applied mechanical stress. A) Under biaxial stress, the atomic layout remains a hexagonal shape. B) Under uniaxial stress, the hexagon deforms, and the strain in the x-direction differs from the strain in the y-direction. © [2010] American Institute of Physics, reprint with permission from [M. Chu et al., "Simulation of AlGaN/GaN high-electron-mobility transistor gauge factor based on two-dimensional electron gas density and electron mobility", J. Appl. Phys., vol. 108, pp. 104502, Fig. 6, November 2010]

The primitive translation vectors and basis vectors in rectangular coordinates are calculated the same way as under biaxial stress. Figure 4-3B shows that under uniaxial stress, the bond length between the central atom to atom 1 differs from the bond length between the central atom to atom 2 or atom 3. The original symmetry is broken, and therefore, the expressions of Hamiltonian matrix elements derived in [73] need to be regenerated, following a standard tight-binding method with the two-center approximation.
as described in [102]. All of atom 1, 2 and 3, as shown in Figure 4-3B, are still considered to be the nearest-neighbors to the central atom. During our derivation, it is found that besides the bond length and bond angle, the expressions of $g_0$, $g_1$, $g_2$, and $g_3$ in [73] also change. The reciprocal lattice, under uniaxial stress, is not hexagonal in shape. The effective mass should be calculated along directions based on the new reciprocal lattice vectors.

Stress-induced band warping is determined by, first, whether the applied stress is along a high-symmetric direction, and second, whether there is strong subband interaction between the conduction band and any other subband. In this work, we study the effect of biaxial stress and uniaxial stress along [11\bar{2}0] and [10\bar{1}0] directions. Although these types of stresses slightly alter the wurtzite crystal symmetry, we expect little change in electron effective mass, and thus electron mobility. This is because GaN has a large bandgap, and has no energetically adjacent conduction bands.

4.2.3 Simulation Uncertainty

In this work, the simulation uncertainty is investigated by considering various elastic stiffness constants and piezoelectric coefficients of GaN and AlN listed in literature. The uncertainty arising from the tight-binding parameters is neglected, since these parameters are achieved from an empirical tight-binding method that is considered to be accurate.

To sum up this section, we expect that both the 2DEG sheet carrier density and the electron mobility have a weak dependence on external mechanical stress, leading to a small gauge factor for the AlGaN/GaN HEMT.
4.3 Results and Discussion

Figure 4-4 shows the percentage change of 2DEG sheet carrier density versus [11\bar{2}0] tensile stress. An increase in $n_S$ ranging from 0.09% to 1.4% for 500MPa can be achieved depending on the coefficients’ value used in the simulation. This small enhancement matches our expectation due to the fact that the additional piezoelectric polarization in AlGaN and GaN layers mostly cancel each other out.

The stress effect on the electron effective mass along the longitudinal, transverse, and out-of-plane directions are calculated and the results are plotted in Figures 4-5A-C, respectively. Here we consider the [11\bar{2}0] direction to be the channel direction. Therefore, the longitudinal, transverse and out-of-plane directions refer to the [11\bar{2}0],
[10\bar{1}0], and [0001] direction, respectively. The shaded areas in the plots include all possible simulation results considering simulation uncertainties. Without stress, the longitudinal, transverse, and out-of-plane effective masses are 0.198m₀, 0.197m₀, and 0.189m₀, respectively, which agree with the results in [73]. For longitudinal effective mass, biaxial stress has a slightly larger effect than uniaxial stress (~3%/500MPa under biaxial stress comparing to ~1.5%/500MPa under longitudinal stress). Similarly, transverse and out-of-plane effective mass also have a larger change under biaxial stress. For all types of stress, however, the changes in electron effective mass of GaN are much smaller than those of Si (~15%/500MPa under <110> uniaxial stress[17]). This is because the subband splitting, which is an important factor affecting electron effective mass in Si, does not exist in GaN. Si is an indirect-bandgap material with the conduction band minimum located near the X point, leading to six degenerate conduction bands. When stress is applied, the Δ₆ conduction bands split into Δ₂ and Δ₄ valleys, and the splitting causes electrons to repopulate. Since the conductivity effective mass of these sub-bands are different (0.415m₀ for Δ₄ valley comparing to 0.19m₀ for Δ₂ valley), the total average effective mass changes depending on the amount of band splitting. The absence of band splitting and carrier repopulation in GaN causes the electron effective mass and thus mobility to only depend on conduction band warping, which is proved to be small through tight-binding calculations.

Combining the variation of 2DEG sheet carrier density and electron mobility, the stress-induced change in channel resistance of an AlGaN/GaN HEMT is plotted in Figure 4-6. Simulation uncertainties are included. The simulation result is compared to the experimental result presented in [49], in which repeatable gauge factors were
obtained after eliminating parasitic charge trapping effects. The simulated gauge factor is determined to be \(-7.9\pm5.2\), compared to \(-2.5\pm0.4\) in [49] while the values published in literature range from -4 to -40,000, as listed in Table 4-1. The wide range of gauge factors listed in literature is considered to be a result of the trapping effect occurring over the elapsed time of measurements. Our result also agrees with the gauge factors of bulk GaN reported in [44, 103-104] with little variation (-1 to -3.6) that indicates negligible trapping effect. Comparing the simulation result with the experimental result of [49], the best fit set of elastic stiffness constants and piezoelectric coefficients used in simulation were determined to be $C_{ij}$(GaN) [105], $C_{ij}$(AlN) [106], $e_{ij}$(GaN) [103], and $e_{ij}$(AlN) [107], as listed in Table 4-2 and Table 4-3.

### 4.4 Conclusion

Stress was incorporated into a sp$^3$d$^5$-sp$^3$ empirical tight-binding method by recalculating the atom locations, the reciprocal lattice, and consequently the bond length, bond angle and the Hamiltonian matrix elements. The tight-binding calculation results indicate small change in electron effective mass and thus mobility. External mechanical stress generates additional piezoelectric polarization in both AlGaN and GaN layers that cancel with each other. Therefore, stress has little impact on the 2DEG sheet carrier density. Combining the stress-varied 2DEG sheet carrier density and electron mobility, the gauge factor of AlGaN/GaN HEMT device was calculated to be \(-7.9\pm5.2\). This indicates a small stress dependence on the HEMT device channel resistance. The best fit set of elastic stiffness constants and piezoelectric coefficients of GaN and AlN was determined by comparing the simulated and measured gauge factors.
Figure 4-5. Change of electron effective mass under externally applied mechanical stress. A) Longitudinal stress. B) Transverse stress. C) Biaxial stress. © [2010] American Institute of Physics, reprint with permission from [M. Chu et al., “Simulation of AlGaN/GaN high-electron-mobility transistor gauge factor based on two-dimensional electron gas density and electron mobility”, J. Appl. Phys., vol.108, pp.104502, Fig.7 (a), November 2010].
Figure 4-5. Continued.
Figure 4-6. Change of GaN HEMT resistance ($R_{TOT}$) under longitudinal stress. Symbols represent experimental change in $R_{TOT}$ [49] with uniaxial stress. © [2010] American Institute of Physics, reprint with permission from [M. Chu et al., “Simulation of AlGaN/GaN high-electron-mobility transistor gauge factor based on two-dimensional electron gas density and electron mobility”, J. Appl. Phys., vol.108, pp.104502, Fig.8, November 2010].
Table 4-1. Gauge factors of GaN HEMTs and bulk GaN published in literature.

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<tr>
<th>Ref.</th>
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<th>$\varepsilon$ (%)</th>
<th>$\sigma$ (MPa)</th>
<th>Method of Stressing</th>
</tr>
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<td>0.114</td>
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<td>[43]</td>
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<tr>
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<td>38.7</td>
<td>9.4</td>
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<td>AlN</td>
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CHAPTER 5
EFFECT OF STRESS ON GAN HEMT GATE LEAKAGE

5.1 Motivation

Great potential for high-power wide-band application has been demonstrated by the AlGaN/GaN HEMT, though its overall performance is limited by reliability issues [100, 109]. The degradation phenomena of HEMT devices, such as current collapse, $V_T$ shift, gate lag, drain lag, transconductance frequency dispersion and barrier breakdown, have been attributed to either hot electron or the inverse piezoelectric effects [100].

The degradation mechanisms include both electronic mechanisms as well as mechanical stress. In the theory of the hot electron effect, the high electric field present in the GaN channel enables electrons to gain enough energy to overcome the potential barrier and enter the AlGaN where they are trapped by the donor-like traps. These traps may occur at the AlGaN surface, in the AlGaN bulk region, as well as at the AlGaN/GaN interface. The trapped negative charge acts as a virtual gate [110], which decreases the channel carrier density and consequently results in a decrease of drain current and a possible increase of threshold voltage. In the theory of inverse piezoelectric effects, additional mechanical strain is generated in the AlGaN layer when an electric bias is applied. This mechanical strain in addition to the lattice mismatch-induced strain in the AlGaN layer can exceed the critical mechanical yield stress limit of AlGaN. This fracture is postulated to result in a sudden device degradation inducing a much larger gate current [51]. To validate this hypothesis, a mechanical bending experiment has been done on GaN HEMTs under high reverse gate bias with zero potential drop between the source and drain [52]. An increase of gate current and a decrease of the critical breakdown voltage with tensile stress were observed.
As important as researching the catastrophic degradation mechanisms of HEMTs is, investigating the pre-degradation device behavior such as the reverse-biased gate leakage current can provide fundamental understanding of the physics behind gradual degradation. It has been proposed that the defects in the bulk AlGaN barrier, at the AlGaN surface, or at the AlGaN/GaN interface are likely to contribute to the gate leakage current [111-112]. During device operation, the AlGaN layer has additional strain induced by the inverse piezoelectric effect, which may shift the defect energy levels. This change in defect characteristics is expected to affect the gate leakage current and device reliability. To better predict GaN HEMT performance and reliability, it is important to understand the effects of mechanical strain on the HEMT gate leakage current.

In this chapter, a comprehensive study of the gate leakage mechanisms in the reverse-biased GaN HEMT is presented. Mechanical stress is incorporated into the model in order to simulate the stress-altered gate leakage current.

**5.2 Gate Leakage Mechanisms**

In this section, several potential leakage mechanisms in the reverse-biased GaN HEMT are modeled, as a function of electric field in the AlGaN barrier and temperature. By comparing with the experimentally observed gate current density, the dominant gate leakage mechanism is determined. The effects of external stress on the electron out-of-plane effective mass, AlGaN electric field, and defect energy levels are investigated. Combining these factors, the stress sensitivity of the gate current at various electric field strengths and temperatures is modeled and analyzed.
5.2.1 Literature Review

Several leakage mechanisms have been proposed in the literature to explain the GaN HEMT gate current at various temperature and field strength conditions. Zhang et al. [113] noted that direct tunneling of electrons from the metal gate into the GaN bulk dominates the gate current measured at low temperature (<130K), while the gate current measured at room temperature or above follows the Poole-Frenkel Emission (PFE) trend. Mitrofanov et al. [114] and Yan et al. [115] also brought up a similar conclusion that PFE dominates the room temperature gate leakage. Karmalkar et al. [111] developed a bulk defect-assisted tunneling gate leakage model. In their model, the electrons undergo two thermal-assisted direct tunneling processes: from the gate to the trap and from the trap to the bulk GaN. They were able to reproduce their experimental results on various devices by using different sets of parameters including the defect level, defect density, and the Schottky barrier height. Sathaiya et al. [112] proposed a similar two-step thermal-assisted tunneling model to be the dominant leakage mechanism in the GaN HEMT. Despite many models, only a few of them [115] considered the backward-current which is essential in order to balance the forward current to properly satisfy the zero net current at zero-bias equilibrium condition.

Summarizing the literature findings, a single leakage mechanism dominating the GaN HEMT gate current at all conditions does not exist. The dominant leakage mechanism depends on temperature, gate bias, and device quality. In the following, several candidate leakage mechanisms are examined before the dominant one is determined for our devices under our experimental conditions. The backward-current will be included in our model to study the stress dependence of the gate leakage current.
Figure 5-1. Schematic illustrations of the gate leakage process in a reverse biased GaN HEMT. A) Fowler-Nordheim tunneling. B) Thermionic Field Emission.

Figure 5-2. Relation between the gate bias and the vertical electric field in the 18nm thick Al_{0.26}Ga_{0.74}N layer. This relation has been confirmed by both TCAD simulation and experimental measurements.

5.2.2 Direct Tunneling

In this work, the direct tunneling takes into account the Fowler-Nordheim tunneling (FN) and Thermionic Field Emission (TFE). Figure 5-1 schematically illustrates the
direct tunneling processes. To simulate this leakage current, the classical models for FN and TFE are used. These models can be expressed analytically as Eq. (5-1) for the FN tunneling [116] and Eq. (5-2) through (5-4) for the TFE [111], respectively.

\[ J = \frac{q^2 \left( m_e / m^* \right)}{8\pi \hbar \phi_B} E^2 \exp \left( -\frac{8\pi \sqrt{2m^*(q\phi_B)^2}}{3q\hbar E} \right) \]  

(5-1)

\[ J = \frac{qA^* T}{k} \int_0^{\phi_b} f_{FD} (\phi) P(\phi) d\phi \]  

(5-2)

\[ f_{FD} = \frac{1}{1 + \exp \left( \frac{\phi_B - \phi}{kT/q} \right)} \]  

(5-3)

\[ P = \exp \left( -\frac{8\pi \sqrt{2m^* q}}{3\hbar E} \phi^{3/2} \right) \]  

(5-4)

Here, \( q \), \( m_e \), \( h \), \( k \), and \( A^* \) are the electron charge, the free electron mass, the Planck constant, the Boltzmann constant, and the effective Richardson constant, respectively. \( E \) is the electric field strength in the AlGaN layer. \( m^* \) is the out-of-plane effective mass of electrons inside AlGaN. \( f_{FD} \) is the Fermi-Dirac distribution function of electrons on the metal side. \( \phi_B \) is the Schottky barrier height between the metal gate and the AlGaN, obtained from Eq. (5-5) considering the barrier lowering due to image force and band gap narrowing [111]. The values of \( \phi_{B0} \), \( \gamma_1 \), and \( \gamma_T \) are 1.4eV, 0.4, and 2.4\times10^{-4} \text{ V/k} for AlGaN [111].

\[ \phi_B = \phi_{B0} - \gamma_1 \sqrt{\frac{q}{4\pi \varepsilon}} \sqrt{E - \gamma_T T} \]  

(5-5)

In order to compare simulation and experimental results, an accurate transformation from the applied gate voltage to the vertical electric field in the AlGaN
barrier is required. For this purpose, a Sentaurus TCAD model is developed and the electric field at various bias conditions is simulated. In addition, high-frequency (capacitance-voltage) CV measurement and threshold voltage measurement are carried out to confirm the voltage-field relation [117]. The result is shown in Figure 5-2. It indicates that the AlGaN electric field under the gate region begins to saturate at \(|V_g|=1.6\text{V}\). Beyond this threshold voltage, the 2DEG is depleted and only the electric field at the edge of the gate increases further. To avoid ambiguity in future discussion, we defined “above threshold” as the condition at which the 2DEG exists and the device is on. The “below threshold” is defined as the condition at which the 2DEG is completely depleted and the device is off.

Figure 5-3. Simulation results of the FN tunneling current and the TFE current at room temperature.
Figure 5-3 shows the simulated direct tunneling current and the experimental measured gate current at room temperature. The result shows that the direct tunneling currents are several orders smaller than the experimental observation until at least 2.5MV/cm. This is expected since the AlGaN layer (18nm) is too thick for the electrons to have a high tunneling rate. In addition, the Schottky barrier height (~1.4eV) is unlikely to result in a high thermal emission rate at room temperature.

As a result, direct tunneling is not the dominant leakage mechanism in our devices when biased above the threshold ($V_g > -1.6V$). At below threshold, there can be a direct tunneling path at the edge of the gate once the edge electric field is high enough.

5.2.3 Bulk Trap-Assisted Leakage

![Schematic illustration of the 2-step bulk trap-assisted leakage process.](image)

This work adopts Fleischer's two-step leakage model [118] and develops it to incorporate the thermal contribution in step 2. In the first step of our model, the electrons tunnel from the metal gate to the trap level through direct tunneling or thermal-
assisted direct tunneling. In step 2, electrons escape from the trap into bulk GaN through direct tunneling, Poole-Frenkel emission [119], or Phonon-assisted tunneling [120-121]. The complete leakage process is shown schematically in Figure 5-4. The tunneling (emission) rates of step 1 and 2 are calculated from Eq. (5-6) and (5-7).

\[
R_1 = C_i N_i f_{FD} (1 - f) P_1 \tag{5-6}
\]

\[
R_2 = C_i N_i f P_2 \tag{5-7}
\]

Here, \(N_i\) is the bulk defect density, \(f\) is the probability that the defect level is filled with an electron, \(P_1\) and \(P_2\) are the tunneling (emission) probability, and \(C_i\) is given by

\[
C_i = \left(\frac{m^*}{m_e}\right)^{5/2} \left(\frac{8E_i^{3/2}}{3h\sqrt{E_T - E_i}}\right) \tag{5-8}
\]

where \(E_T\) is the defect level and \(E_i\) is the total energy of an electron (0.2eV [118]). \(P_1\) is calculated following the standard direct tunneling expression

\[
J = \frac{q^2}{8\pi \hbar \phi_0} \left(\frac{m_e}{m^*}\right) E^{-2} \exp\left(-\frac{8\pi\sqrt{2m^*q}}{3hE} \left(\phi_B^{3/2} - \phi_0^{3/2}\right)\right), \tag{5-9}
\]

and \(P_2\) is calculated using either the FN tunneling model, the classical Poole-Frenkel emission model, or the phonon-assisted tunneling model developed by Pipinys et al.[120]. At steady state, \(R_1\) should equal \(R_2\). After a straightforward mathematical derivation, the tunneling rate \(R\) is obtained,

\[
R = N_i \left(\frac{1}{C_i f_{FD} P_1} + \frac{1}{C_i P_2}\right)^{-1}. \tag{5-10}
\]

The overall gate current density is then calculated by integrating \(R\) over the thickness of the entire AlGaN barrier.

\[
J = \frac{q}{E} \int_{\phi_B}^{E_d} R(\phi) \, d\phi \tag{5-11}
\]
In the current model, a uniform defect distribution is assumed across the AlGaN barrier. The AlGaN potential profile is assumed to be triangular, which is reasonable for devices biased above threshold. We also considered only one single effective defect level as a fitting parameter.

Figure 5-5 shows the calculated and experimental gate current density at room temperature, with \( N_t=5 \times 10^{17} \text{ cm}^{-3} \) and \( E_T=0.82 \text{ eV} \). The value of \( E_T \) significantly affects the resulting current magnitude. In fact, \( E_T \) has opposite effects on \( P_1 \) and \( P_2 \). With small \( E_T \), the energy difference between the metal gate Fermi level and the defect level is large, and the first step of electrons tunneling from the metal gate into the defect level is unlikely to happen. With large \( E_T \), the energy difference between the defect level and the AlGaN conduction band is large, and the step two probability of electrons
undergoing PFE or PAT becomes smaller. The value of $E_T=0.82$eV was obtained by trying to match the two step model and the experimental results within the same order of magnitude, under a reasonable defect density $N_d=5\times10^{17}$/cm$^3$. Under this condition, it is found that the calculated current density does not depend on the chosen mechanism for the $P_2$ step. This indicates that the first step of electrons tunneling from the metal gate into the defect level limits the bulk trap-assisted leakage current.

Regardless of what leakage mechanism for step two and fitting parameters are chosen, a good match between the model and experimental results is unachievable. This suggests that the bulk trap-assisted tunneling mechanism is not the dominant leakage mechanism in our GaN HEMT devices.

5.2.4 Poole-Frenkel Emission from Surface States

It has been proposed in literature that the donor-like surface states can trap hot-electrons and act as a “virtual gate”. Here, these surface states are considered to participate in the gate leakage process through Poole-Frenkel Emission in the reverse-biased GaN HEMT.

This work develops a surface-state-related leakage mechanism, as shown schematically in Figure 5-6. $J_{PF}$ stands for the forward Poole-Frenkel Emission current and $J_{back}$ stands for a backward current. Since a non-zero electric field exists at zero gate bias leading to a non-zero forward current, it is essential to include the $J_{back}$ in the model to ensure zero net current at zero applied gate bias at equilibrium. At any bias, the net gate current is obtained from the difference between the forward and backward currents, $J_{PF}-J_{back}$.

The forward current is modeled by a modified Poole-Frenkel Emission mechanism. The classical Poole-Frenkel equation has the form [119]
\[ J_{pf} = CE \exp \left( -\frac{E_T - \Delta \phi_T}{kT} \right) \]  \hspace{1cm} (5-12)

where \( \Delta \phi_T = \beta \sqrt{E} = \sqrt{\frac{q^2 E}{\pi\varepsilon_0\varepsilon_{AlGaN}}} \) represents the defect barrier lowering due to the electric field in the AlGaN layer. \( C \) is a constant related to the electron mobility and interface defect density [122]. It is important to note that it is the high-frequency permittivity that should be used as the AlGaN permittivity [123] in the barrier lowering term. From \( \varepsilon_{AlN} = 4.6 \) and \( \varepsilon_{GaN} = 5.3 \), the calculated permittivity for Al\(_{0.26}\)Ga\(_{0.74}\)N is 5.1. Other parameters have their usual meanings.

Figure 5-6. Schematic illustration of the Poole-Frenkel Emission process from the surface states. The net gate current is the difference between the forward Poole-Frenkel current and the backward electron “diffusion” current.
However, it is well known that the slope of a classical Poole-Frenkel model, \( \log(J/E) \) vs. \( E^{1/2} \), often deviates from the experimental observations [124]. A more generalized Poole-Frenkel Emission model has been proposed as [123]

\[
J_{PF} = CE \exp \left( -\frac{E_T - \Delta \phi_T}{r kT} \right)
\]  

(5-13)

Here, the parameter \( r \) accounts for compensation effects between the donor-like defect states and any possible acceptor states. It equals 1 for full compensation and 2 for no compensation. Depending on how heavy the compensation is, \( r \) varies between 1 and 2. In this work, the \( r \)-parameter is treated as a fitting parameter to best fit our experimental observations.

Figure 5-7. Modeling results of the Poole-Frenkel Emission from surface states at various temperatures. The experimental results are also shown for comparison. The inset shows the J vs. E in the linear scale.
For the backward current, its physical mechanism is still unclear. It possibly relates to the bulk-defect-assisted electron hopping from the AlGaN/GaN interface back to the AlGaN surface states, as shown in Figure 5-6. It is likely to have a “diffusion” type of behavior due to the density gradient of the trapped electrons inside the AlGaN. For the modeling purpose, we adopt the form of tunneling current proposed by Yan [115]. Instead of using the classical direct tunneling model, we incorporated a parameter $C'$ in the pre-exponential term of Eq. (5-14), which satisfies $J_{\text{back}} = J_{PF}$ at $V_g=0V$. Since $J_{PF}$ increases significantly once $V_g \neq 0$ and $J_{\text{back}}$ becomes negligible, estimating $J_{\text{back}}$ from a rough model should not affect the overall calculation.

$$J_{\text{back}} = C' \exp \left( -\frac{8\pi \sqrt{2m^*(q\phi)^3}}{3qhE} \right)$$  \hspace{1cm} (5-14)

Combining the forward and backward current, the simulated $\log(J/E)$ vs. $E^{1/2}$ at various temperatures is shown in Figure 5-7, together with the experimentally measured results for comparison. The inset shows the $J$ vs. $E$ in the linear scale. Good agreement between the model calculation and experiment is achieved by using the set of fitting parameters as noted in Table 5-1. The uncertainties of the fitting parameters are also listed in Table 5-1. The $r$-parameter determines the slope of the Poole-Frenkel plot and its uncertainty is calculated based on a 10% slope variation. $E_T$ determines the temperature dependence of the modeled gate leakage current. Its uncertainty is determined at the moderate electric field (Poole-Frenkel dominated) region, from the condition that the simulated temperature dependence has less than 10% deviation from the experimental observation. The variations of $r$ and $E_T$ alter the value of $C$ as shown in Table 5-1. The value of the $r$-parameter (1.25) indicates that a certain level of
compensation exists. It is also interesting to note that the fitting parameter $E_T=0.49$ closely agrees with our experimentally extracted $E_T=0.5$. Based on the above discussion, it is concluded that the dominant gate leakage mechanism in our GaN HEMTs is the Poole-Frenkel Emission from the surface states.

Table 5-1. The Poole-Frenkel Emission fitting parameters.

<table>
<thead>
<tr>
<th>$r$</th>
<th>$E_T$</th>
<th>$C$</th>
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<tbody>
<tr>
<td>1.25 (±0.06)</td>
<td>0.49 (±0.04)</td>
<td>7.3×10^{-6} (0.22×10^{-6}~25×10^{-6})</td>
</tr>
</tbody>
</table>

5.3 Effects of Stress on Gate Leakage

In this section, external stress is incorporated into the previously developed gate leakage model to study the stress-altered gate current. In the model of Poole-Frenkel Emission from surface states, stress can affect the gate current through the electron out-of-plane effective mass, the AlGaN electric field, the defect energy level, and the $r$-parameter.

5.3.1 Stress-Dependent Parameters

We used the $sp^3d^6-sp^3$ tight-binding model developed in Chapter 4 to calculate the change of electron out-of-plane effective mass under both uniaxial and biaxial stress. In the experiment, the uniaxial stress is induced by wafer bending, and the biaxial stress is induced by the inverse piezoelectric effect when gate bias is present. Figure 5-8 shows the tight-binding calculation results for both uniaxial and biaxial stress. It is observed that the electron out-of-plane effective mass has negligible change under both stresses (<0.5% per 400MPa).

Stress causes variation in the AlGaN polarization due to the piezoelectric effect, leading to a change in the electric field strength. Following the discussion in Chapter 4, this additional piezoelectric polarization can be calculated by $P_{PE,mach}^{PE} = e_{ij} \cdot \varepsilon$, where $e_{ij}$ is
the piezoelectric constants and $\varepsilon$ is the strain. The simulation results for both uniaxial and biaxial stress are shown in Figure 5-9. Approximately 0.7% and 1.4% change in polarization is predicted for 400MPa uniaxial and biaxial stress, respectively. This observation indicates a weak stress dependence of the AlGaN electric field.

Figure 5-8. Change of the electron out-of-plane effective mass under uniaxial and biaxial stress.

Stress has been proposed to shift the defect energy level by changing the atom-defect bond angle and bond length [125]. It was observed that both tensile and compressive stresses decreases Pb$_1$ (or Pb$_2$) defect levels for Si MOSFETs, resulting in an increase of gate leakage current [125]. For GaN HEMTs, our experimental results in Figure 5-10 show that tensile stress increases gate current, while compressive stress decreases gate current. This can be explained qualitatively with Figure 5-11, taking the N-vacancy as an example. As mentioned in Chapter 4, approximately 2.8GPa biaxial stress is present in the AlGaN layer due to lattice mismatch. Compared to the
unstrained lattice, the bond angle $\Theta_1$ decreases and $\Theta_2$ increases, and the bond length $L_1$ decreases and $L_2$ increases. The defect in the AlGaN becomes less stable under this large stress, and its energy level shifts up towards the conduction band. When a tensile wafer bending stress is applied, a similar trend of bond angle and bond length variation is expected. It adds to the effect of biaxial stress and shifts the defect level further up. In contrast, a compressive wafer bending stress tends to relax the strain from the lattice mismatch, therefore results in a downward shift of the defect level towards its original state. Since the gate current exponentially depends on the defect level, a decrease (or increase) of the defect level from tensile (or compressive) stress increases (or decreases) the gate current. In this work, $\Delta E_T$ is treated as a fitting parameter between simulation and experiment. A more rigorous theoretical model is yet to be developed for a quantitative prediction of the stress-altered defect level.

Figure 5-9. Change of polarization in the AlGaN layer under uniaxial and biaxial stress.
Figure 5-10. Experimentally measured gate leakage current change under uniaxial tensile and compressive bending stress. The current is measured under $V_G = -0.25V$.

The $r$-parameter also varies with stress, due to the shift of the defect level as shown in Figure 5-12. Under tensile stress, the defect level shifts towards the conduction band, resulting in a higher probability of electron emission from the defect state into the conduction band. This indicates weaker compensation and thus a higher $r$ value. In contrast, when compressive stress is applied, the defect level shifts downwards, resulting in a smaller probability of emission. This indicates stronger compensation and thus a smaller $r$ value.
5.3.2 Results and Discussions

Incorporating the above discussed factors into the model of Poole-Frenkel Emission from surface states, the change in the GaN HEMT gate current under uniaxial bending stress is calculated and shown in Figure 5-13. At room temperature, a close match between the simulation and experimental results at various electric fields, $E_{AlGaN}$, is obtained by fitting $\Delta E_T = 1.6 \pm 0.3$ meV/GPa and $\Delta r = 0.028 \pm 0.004$ /GPa. The uncertainties of $\Delta E_T$ and $\Delta r$ are determined based on the condition that the modeled gate current change has less than 10% deviation from the experimental results including error bars. The smaller stress sensitivity of the normalized gate leakage current change in Figure 5-13 indicates a weaker stress dependence at higher reverse gate bias. It also shows that the stress dependence of the gate current decreases with increasing temperature. The Poole-Frenkel Emission barrier is lowered at higher gate bias, and the electron thermal energy increases at higher temperature. Both effects indicate a stronger electron emission and weaker compensation. And therefore, the stress-altered $r$-parameter (representing compensation) has smaller effect compared to the low bias (or lower temperature) case where the compensation effect is more important.

5.4 Conclusion

In this chapter, several possible gate leakage mechanisms have been examined and the dominant leakage in the reverse-biased GaN HEMT (above threshold) is determined to be the Poole-Frenkel Emission from AlGaN surface states. Its stress dependence is investigated through the stress-altered electron out-of-plane effective mass, the AlGaN electric field, the defect level, and the $r$-parameter. It increases
(decreases) under tensile (compressive) stress, with less than 2% change per 100MPa stress. For the GaN HEMT biased below threshold, the electron direct tunneling from the gate edge becomes important, which is expected to have negligible stress dependence.

Figure 5-11. Schematic illustrations of the defect bond angle and bond length variation, and the defect level shift under lattice mismatch and wafer bending stress.

Figure 5-12. Schematic illustration of the effect of externally applied mechanical stress on the $r$-parameter.
Figure 5-13. Simulation results for the stress-altered GaN HEMT gate leakage current at various temperatures. The simulation is based on the model of Poole-Frenkel Emission from surface states. The room temperature experimental results are also shown.
CHAPTER 6
DFT CALCULATION FOR GAN

The density functional theory (DFT) calculation is investigated and applied to bulk GaN. This chapter describes and discusses the DFT calculation procedure to obtain the GaN band structure with a correct band gap. In order to investigate the effects of strain on the GaN HEMT gate leakage current, a DFT strategy for defect level calculation is then explored.

6.1 DFT Introduction

6.1.1 Basic Concept of DFT

DFT is a quantum mechanical method for calculating electronic structures of material systems. It is especially popular in the investigation of ground-state properties of relatively large systems whose supercell typically contains ~100 atoms. The key idea behind DFT is to solve the Schrödinger Equations and view the solutions as a functional of electron density, instead of the spatial coordinates of each individual electron [126].

The classical Schrödinger Equation is described as

$$\left[ \frac{\hbar^2}{2m} \sum_{i=1}^{N} \nabla^2_i + \sum_{i=1}^{N} V(r_i) + \sum_{i=1}^{N} \sum_{j=i}^{N} U(r_i,r_j) \right] \psi = E\psi \quad (5-15)$$

The three terms inside the bracket represent the kinetic energy of each electron, the interaction between each electron and the nuclei, and the electron-electron interaction. For a system containing N electrons, the full solution is a function of 3N coordinates. As a result, a rigorous solution of the Schrödinger Equation becomes a formidable task for practical material systems that have more than tens of electrons. In addition, the factors that we are actually interested in and can be physically measured are not the individual electron wave functions, but the possibility that a set of electrons
are present at a real space point. This is directly related to the electron density described as \( n(r) = 2 \sum_i \psi_i^*(r) \psi_i(r) \). By solving the Schrödinger Equation using a functional of the electron density, the solution becomes only 3-dimensional.

The density functional theory is based on two fundamental mathematical theorems proved by Kohn and Hohenberg [127]. (1) "The ground-state energy from Schrödinger’s equation is a unique functional of the electron density." (2) "The electron density that minimizes the energy of the overall functional is the true electron density corresponding to the full solution of the Schrödinger equation." Based on these theorems, there exists a unique ground-state electron density corresponding to a specific ground-state wave function. As a result, the Schrödinger equation can be solved by finding the electron density that only depends on three spatial coordinates, rather than the electron wave function, which depends on 3N variables.

To solve for the right electron density, Kohn and Sham derived a set of equations in 1965 [128], in which each equation involves only one electron. The Kohn-Sham equation is expressed as

\[
\left[ \frac{\hbar^2}{2m} \nabla^2 + V(r) + V_H(r) + V_{XC}(r) \right] \psi_i(r) = \varepsilon_i \psi_i(r)
\]  

(5-16)

The three potentials inside the bracket represent the electron-nuclei interaction, the Hartree potential, and the exchange and correlation potential. The Hartree potential describes the Coulomb repulsion between a single electron and the total electron density. Since the total electron density also has the contribution from the electron itself, the unphysical interaction between this electron and itself is included in the \( V_H \) term. As a result, researchers use the \( V_{XC} \) term to correct this self-interaction fault. Formulating
and choosing a physically reasonable $V_{xc}$ theme is of particular importance for a successful description of material system by DFT. Developing the exchange and correlation functional remains a hot topic in material and chemistry science. The most popular ones are the Local Density Approximation (LDA) [128-132], Generalized Gradient Approximation (GGA) [133-136], LDA+U method [137-138], and Hybrid Functional method [139-143].

Figure 6-1. The self-consistent procedure for a standard DFT calculation.

The Kohn-Sham equations must be solved self-consistently [144] as shown in Figure 6-1. A trial electron density defines the Kohn-Sham equations to solve for the single-electron wave functions. The resulting wave functions are used to calculate a
new electron density. If the difference between the initial density and the calculated density is within a pre-defined stopping criterion, then this result is determined to be the right ground-state electron density. The corresponding energy is the true total energy of the system. If the two densities are too different, then the trial electron density will be modified in a pre-defined way. This will serve as the new trial electron density and the whole process repeats until the stopping criterion is met.

6.1.2 Why Choose DFT

There are several modeling methods capable of calculating the electronic structure of a set of atoms. These methods include the *ab-initio* (such as DFT, molecular dynamic), semi-empirical (such as semi-empirical pseudopotential), or empirical (such as tight-binding and k·p method) methods. In Chapter 4, the tight-binding method was used to calculate the stress-altered GaN band structure and electron effective mass. The calculation process is relatively straightforward and the stress effects can be physically previewed through the change of bond length and bond angle between neighboring atoms, which results in a change in the atom-atom interaction. However, the tight-binding calculation requires several input parameters such as the on-site one-center and nearest-neighbor two-center integrals. These parameters need to be obtained either from experiment or first principle calculation. There are not available defect-related parameters for GaN, and therefore the tight-binding method is not able to provide information about the defect electronic structure of GaN.

In this work, the DFT method was chosen to investigate the feasibility of defect energy calculation due to the following reasons: (1) DFT is a first principle calculation. Ideally, it does not depend on any empirical inputs. (2) DFT is computationally more efficient than the more rigorous first principle methods such as the Hartree Fock
calculation. Thus, it is capable of dealing with practical systems that contains hundreds of electrons. (3) It is straight forward to incorporate external stress into the DFT model by manually modifying atom locations. (4) It is also straight forward to put defects into the system, regardless of what type the defect is and where it occurs. (5) There are several available simulation packages (such as SeqQuest, Socorro, and VASP) to make DFT user-friendly. Researchers may perform their own calculations using such simulation packages without full understanding of the derivation, parameterization, and computation algorithm for the DFT method.

The DFT calculation delivers useful information about material systems. It provides the true lattice structure by relaxing the atomic sites until a minimum energy is obtained. It can also predict what types of defects are more likely to form by computing the energy difference between systems with and without defects. This energy difference is called the “defect formation energy”. The lower the formation energy, the easier it is for this particular type of defect to form. The DFT calculation also provides the electronic band structure of the material, from which the defect levels and density of states can be derived. In this work, the defect energy level is the most desired property that is important for GaN HEMT gate leakage simulation.

6.1.3 DFT Calculation Procedure Using VASP

In this work, DFT calculation is executed using Vienna Ab-initio Simulation Package (VASP) [145-146]. “VASP is a complex package for performing ab-initio quantum-mechanical molecular dynamic simulations using pseudopotentials or the projector-augmented wave (PAW) method and a plane wave basis set.”, as defined in the VASP user manual [147]. To ensure reliable calculations, four input files must be explicitly provided with proper information included. These four files are named as
POSCAR, POTCAR, KPOINTS, and INCAR. The general DFT calculation in VASP starts up in a procedure as shown in Figure 6-2.

1) — construct supercell (POSCAR)

2) — potential package (POTCAR)

3) — k-points (KPOINTS)

4) — mathematical treatment (INCAR)

Cut-off energy
Stopping criteria
Other options

Figure 6-2. Preparation of VASP input files. The basic input files are the POSCAR, POTCAR, INCAR, and KPOINTS file.

In the POSCAR file, the system lattice geometry is carefully constructed, by defining the basic vectors of the unit cell (or supercell) and the ionic positions. The POSCAR file also provides an optional tag “Selective dynamics”, through which the
users have additional freedom to fix coordinates of certain atoms while allowing others to relax. This option is especially useful for defect calculation in which only ions near the defect site should relax. It is also useful for calculation of systems with external stress applied. In this case, the boundary condition can be satisfied by fixing certain ions.

In the POTCAR file, the proper pseudopotential must be chosen for each element species within the system. VASP uses either the ultra-soft pseudopotential (US-PP) or the PAW method [148]. It was proven that both PAW and US-PP give same results within 0.1% for semiconductors [148].

The KPOINTS file defines the k-mesh in the reciprocal space on which a practical DFT calculation is carried out. The choice of k-points in the Brillouin Zone is very important, because in a DFT calculation a large portion of the computation falls into evaluating the k-space integrals. A denser k-mesh provides more accurate results with the penalty of higher computational cost. There is always a trade-off between accuracy and efficiency. What researchers usually do is to first test the convergence of the number of k-points, and choose the smallest number of k-points that satisfies the convergence requirement.

The INCAR file defines a large number of important parameters that specify a DFT calculation goal (‘what to do’) and determine a particular way to execute the calculation (‘how to do’). These include choosing the plane-wave cut-off energy, the relaxation algorithm, and the calculation stopping criterion.

With the proper POSCAR, POTCAR, KPOINTS, and INCAR files, a DFT calculation can be started. Once the calculation is completed, several output files will
be created providing the relaxed lattice geometry, the computed wave function, the
electron density, the system total energy, and the computation time. These output files
can be the final results of a task, or they can be used as complementary input files for a
further DFT calculation step to solve more complicate problems.

6.2 DFT Calculation for Bulk GaN

In this section, a detailed procedure of the DFT calculation for obtaining the GaN
band structure with correct band gap is discussed. Since the defect levels inside the
GaN band gap is the most essential parameter in a gate leakage simulation, the defect
calculation strategy should be determined in a way that ensures correct band gap.

6.2.1 Standard DFT Calculation

The GaN band structure is calculated using the standard DFT method with the
GGA defined by the PBE functional [134]. The calculation is completed in two steps. In
the first step, a self-consistent DFT calculation is carried out on a k-mesh defined by the
Monkhorst and Pack approach [149]. The chosen number of k-points is 6×6×4 in the k_x,
k_y, and k_z directions, respectively. This set of k-points has been proven to have
converged DFT results for GaN [150-151]. The output wave function file (WAVECAR)
and the relaxed lattice geometry (CONTCAR) from this step will be used as a
complementary input file for the next step. In the second step, a non-self-consistent
DFT calculation is carried out on a set of denser k-points along a high symmetric
direction. The band structure along this direction is then constructed by plotting the
resulting eigen-energies associated with each k-point.

The INCAR, POSCAR and KPOINTS files for unstrained GaN calculations are
attached and described in Appendix A, B and C, respectively. The strained GaN
POSCAR files are obtained by modifying the unstrained basic vectors from [b_x, b_y, b_z] to
[b_x(1+\varepsilon_{xx}), b_y(1+\varepsilon_{yy}), b_z(1+\varepsilon_{zz})], where \varepsilon_{xx}, \varepsilon_{yy}, and \varepsilon_{zz} are calculated by Eq. (4-2) through Eq. (4-6).

Table 6-1. The standard DFT-PBE calculation results for the GaN 4-atom unit cell and 32-atom supercell structures, with and without external stress.

<table>
<thead>
<tr>
<th></th>
<th>Unstrained</th>
<th>Biaxial</th>
<th>Uniaxial &lt;112-0&gt;</th>
</tr>
</thead>
<tbody>
<tr>
<td>4-atom</td>
<td>Done (1 hr)</td>
<td>Done (1 hr)</td>
<td>Done (1 hr)</td>
</tr>
<tr>
<td>32-atom</td>
<td>Done (36 hr)</td>
<td>Done (40 hr)</td>
<td>Done (48 hr)</td>
</tr>
<tr>
<td>‘4’ compares to ‘32’</td>
<td>Same results</td>
<td>Same results</td>
<td>Same results</td>
</tr>
</tbody>
</table>

Calculations based on both a GaN unit cell (2 Ga-atoms and 2 N-atoms) and a 32-atom supercell (16 Ga-atoms and 16 N-atoms) are performed, with and without external stress. The DFT tasks are organized in Table 6-1. Using 8 CPUs simultaneously, the 4-atom calculations took about one hour to finish and the 32-atom calculations took up to two days. From the observation that both input geometries give the same results, it is confirmed that a POSCAR file containing only a single unit cell is able to properly provide the bulk GaN properties. This conclusion indicates that the DFT strategy determined from a 4-atom bulk calculation can be used in the defect calculation with a much larger supercell structure.

Figure 6-3A shows the GaN band structure along the M-\Gamma-A direction obtained from DFT calculation with the GGA functional defined by Perdew, Burke, and Ernzerhof (PBE) [134]. The calculated band gap is 1.81eV, which is much smaller than the experimental observation of 3.4~3.5eV. This is the well-known band gap problem in the standard DFT method, causing by the absence of the derivative discontinuity in the LDA and GGA functionals [152]. In the following sub-section, DFT calculations with the +U correction and the hybrid functional supplement are performed for the purpose of overcoming the band gap problem.
The calculated E-k diagrams for bulk GaN. A) Using the standard DFT-PBE functionals. B) Using the LDA+U method.

6.2.2 Bandgap Correction

The LDA+U method. The LDA and GGA are orbital-independent potentials that treat the semicore states as core states, which tend to over localize the semicore electrons. Therefore, the interaction between the semicore states and the valence band maximum may not be properly described [153], which causes error in the valence band maximum and thus the band gap value. In the LDA+U approach, the electrons are classified into two groups. For the localized electrons, an additional Coulomb repulsion term U is introduced into the exchange and correlation potential, while the delocalized electrons are described by the usual orbital-independent potential in LDA (GGA). The parameter U is a fitting parameter that reproduces the correct bandgap.

The modified INCAR file for +U calculation is shown in Appendix A. The fitting parameter U represents the effective on-site Coulomb interaction, and the parameter J represents the effective on-site Exchange interaction. The GaN band structure calculated from the LDA+U method is shown in Figure 6-3B. The resulting bandgap is 1.83eV. Different choices of U and J parameters end up with similar bandgap. This
indicates that the under-estimation of bandgap does not result from the LDA (GGA) description of semicore states.

**Hybrid functionals.** Hybrid functionals have become increasingly popular in the investigation of defects in solids [154-157]. The core concept of hybrid functionals is to mix the LDA (GGA) exchange potentials with the non-local Hartree-Fork exchange potential while keeping the correlation potential as described by LDA (GGA) [152]. Several forms of hybrid functionals have been proposed in the literature to describe various material systems. In this work, the hybrid functional developed by Heyd, Scuseria, and Ernzerhof (HSE) is used [143]. In the HSE, the short-range exchange potential is formed by mixing PBE with the Hartree-Fock potential. The long-range exchange potential follows the usual PBE potential. This range-separation treatment is instrumental in overcoming the bandgap problem by providing a more realistic potential. However, the partial inclusion of the Hartree-Fock potential tremendously increases the computational cost since it involves four-center integrals.

Due to its high computational cost, instead of starting from the beginning of a problem, the HSE calculation is always performed after a standard DFT calculation step. Obtaining the band structure by HSE involves three steps: (1) A standard self-consistent DFT-PBE calculation, (2) A self-consistent HSE calculation basing on the WAVECAR and the CONTCAR files from step 1, (3) A non-self-consistent HSE calculation along a high symmetry direction. Step 1 is the same DFT-PBE calculation as described before. The INCAR files for step 2 and step 3 are shown in Appendix A. A 4-atom unit cell is used in the HSE calculation.
In the HSE implemented by VASP, a researcher has the freedom of setting the ratio between the PBE and Hartree-Fork exchange potential through the parameter ‘AEXX’. This ratio directly affects the calculated bandgap value and can be treated as a fitting parameter. It is by default 25% Hartree-Fork. Using this default ratio, a bandgap of 2.85eV is obtained. By adjusting the ratio to 31%, we can obtain a 3.47eV bandgap. Table 6-2 summarizes the bandgap values calculated by the DFT-PBE, LDA+U, default HSE, and adjusted HSE functionals. Figure 6-4 shows the GaN band structure along the M-Γ direction calculated by HSE with the ratio of 31%. For the purpose of comparison, the band structures obtained from the tight-binding method discussed in Chapter 4 and from the empirical pseudopotential method [158] are also shown. The calculated HSE bandgap of 3.47eV is in close agreement with the values predicted from the other two methods, as well as the experimental bandgap (3.4~3.5eV).

Table 6-2. GaN bandgaps calculated from the DFT-PBE, LDA+U, and HSE functionals.

<table>
<thead>
<tr>
<th></th>
<th>DFT-PBE</th>
<th>LDA+U</th>
<th>HSE (default)</th>
<th>HSE (AEXX=0.31)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Eg (eV)</td>
<td>1.81</td>
<td>1.83</td>
<td>2.85</td>
<td>3.47</td>
</tr>
</tbody>
</table>

Figure 6-4. The E-k diagrams for bulk GaN. A) Calculated from the DFT-HSE. B) The tight-binding method. C) The empirical pseudopotential method.
It is important to note that the 4-atom HSE calculation for GaN band structure took approximately 3 days to finish by using 8 CPUs simultaneously. The computational cost is 72 times more than the standard DFT calculation.

As a conclusion, the GaN band structure with correct bandgap is obtained by using the HSE method with a mixing ratio of 31%. The setup and the calculation procedure may be employed in the DFT strategy for defect calculation in GaN.

6.3 GaN Defect Calculations

6.3.1 Literature Review

Potential defect levels in GaN HEMT have been extensively studied through various experiment techniques, such as drain current deep level transient spectroscopic (DLTS) [159-165], drain leakage current measurement [166], SIMS characterization [167], and photoionization spectroscopy [168]. A large range of defect levels were observed within the GaN band gap region, as shown in Figure 6-5. However, despite many previous experimental studies, the defect nature and their origins are still not well understood. Recently, Puzyrev et al. proposed a GaN HEMT degradation model in which active defects are generated by hot electrons through dehydrogenation of the H-passivated pre-existing defects [169]. They performed first-principle DFT calculations on candidate defects (N_{Ga}, V_{Ga}, V_{N}^{-} V_{Ga} etc.) and concluded that different defects are responsible for the degradation of HEMTs fabricated under different conditions.

A similar technique can be used in the GaN HEMT gate leakage study. By combining the stressed gate leakage measurement and the DFT calculation, the reverse-biased gate leakage mechanism can be better understood. If both the pre-stressed defect level and the stress-induced level shift match between experiment and
simulation, the corresponding defect and the related leakage model may be confirmed to be the dominant leakage mechanism in the particular GaN HEMT device.

![Graph showing defect levels in GaN HEMT](image)

Figure 6-5. Literature published defect levels observed in GaN HEMTs. The defect levels distribute a wide energy range inside the GaN bandgap. [159-168, 170-171]

### 6.3.2 Test Calculation and Computational Issues

A DFT calculation under the pre-determined HSE strategy was performed to try to obtain candidate defect levels. The chosen candidate defects are nitrogen vacancy, nitrogen-gallium divacancy, and oxygen substituting nitrogen, because these defects are close to the conduction band edge and expected to contribute in Poole-Frenkel Emission. For defect related DFT calculation, a relatively large supercell is commonly used to minimize the interaction between defects in neighboring supercells. For wurtzite GaN, it is recommended to use supercells with 32, 48, 96 or 128 atoms. In this work, a 32-atom supercell was constructed with only one defect inside. For a supercell calculation, employing a single k-point for the Brillouin zone integrations is enough to obtain converged results.
By using 8 CPUs simultaneously, the first step of the standard DFT-PBE calculation took on average 5 days to finish, and the second step of the self-consistent HSE calculation took a tremendously longer time (estimated 24 weeks) to finish. In order to have useful results within a realistic time, more computational facilities and advanced parallelism algorithms are needed for the HSE-based defect calculations. DFT simulation of stress effect on defect energy levels is therefore a potential topic for future work.

6.4 Conclusion

The DFT method was used to accurately calculate the GaN band structure and bandgap. The detailed procedure to obtain the correct bandgap value was discussed. By using the HSE hybrid functional with a mixing ratio of 31%, the GaN band structure with correct bandgap can be achieved. Finally, a DFT calculation strategy for the strain effect on GaN defect level was outlined. This effort is suggested as a possible future study.
CHAPTER 7
SUMMARY AND RECOMMENDATIONS FOR FUTURE WORK

7.1 Summary

This dissertation focused on the piezoresistive properties of field-effect transistors with various device structures (planar MOSFETs, TG FinFETs, HEMTs) and various channel materials (Si, GaN), as well as the effects of mechanical stress on GaN HEMT gate leakage current.

A systematic study of the piezoresistive properties of Si planar MOSFETs and TG FinFETs has been reported. Mechanical stress was applied using four-point and concentric-ring wafer bending setups. It was found that the piezoresistive properties of most FETs vary from the strained characteristics of bulk Si, depending on the surface orientations and channel directions. This is because the surface confinement induces additional subband splitting and consequently alters the carrier population and the scattering rate. Based on the knowledge of planar MOSFETs, the behavior of strained TG FinFET can be understood and predicted.

The piezoresistive property of the GaN HEMT was simulated by considering the strain-altered 2DEG sheet carrier density and electron mobility. It was found that the externally applied mechanical stress has negligible effect on the electron density, due to the cancellation of the stress-induced piezoelectric polarization in both the AlGaN and GaN layers. Strain is incorporated into an $sp^3d^5$ tight-binding model to calculate the mobility change under uniaxial and biaxial stress. The simulation result suggests negligible mobility change due to the fact that the GaN conduction band barely warps. Therefore a small gauge factor is expected for GaN HEMT devices. By comparing with
the experimental results obtained from a technique eliminating the trapping effect, the best fit set of material parameters is determined.

The impact of mechanical stress on the gate leakage current in reverse-biased GaN HEMTs was also investigated. A gate leakage model was proposed, in which the forward current is due to the Poole-Frenkel Emission of electrons from surface states and the backward current is due to the electron “diffusion” from the AlGaN/GaN interface back to the AlGaN surface states. The simulation and experimental results achieved close agreement at various temperatures, by fitting several empirical parameters ($E_T$, $r$, $\Delta E_T$, and $\Delta r$). The gate leakage increases (decreases) with tensile (compressive) stress and its stress sensitivity decreases at larger reverse bias and higher temperature. These results may be explained by the shifting of defect energy level and the altered compensation effect.

Finally, the DFT calculation was performed to obtain the bulk GaN band structure with correct bandgap. The HSE functional with a 31% mixing parameter was determined as the DFT strategy for GaN defect calculation.

7.2 Recommendations for Future Work

The GaN HEMT reliability issues are tightly related to the defects inside the devices. During the GaN HEMT fabrication process, various defects can be introduced into the device. Performing DFT defect calculation on candidate defects can provide useful information such as defect formation energy and defect levels. By combining the gate leakage modeling and the DFT defect calculation, and comparing the simulation results to experiment, the dominant defects and their origins can be better understood.
The GaN HEMTs are conventionally operated under high drain bias. There is a large piezoelectric stress present in the AlGaN barrier, and a large current flows in the channel. Investigation of the impacts of mechanical stress in the high power regime can offer better understanding of GaN HEMT degradation mechanisms.
There are many setting flags that the VASP users can specify based on their own project needs. In this appendix, the INCAR files for the current work using the standard DFT, LDA+U, and HSE methods are list from Table A-1 to Table A-4. A more detail description of these flags can be found in the VASP user manual.

Table A-1. The INCAR file for the self-consistent (SC) calculation step in the standard DFT model.

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<thead>
<tr>
<th>Staring Parameter for this run</th>
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</thead>
<tbody>
<tr>
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<tr>
<td>ICHARG = 2</td>
</tr>
<tr>
<td>LWAVE = .TRUE.</td>
</tr>
<tr>
<td>LCHARG = .TRUE.</td>
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</table>

<table>
<thead>
<tr>
<th># Electronic relaxation</th>
</tr>
</thead>
<tbody>
<tr>
<td>PREC = Accurate</td>
</tr>
<tr>
<td>ENCUt = 500eV</td>
</tr>
<tr>
<td>NELM = 150</td>
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<tr>
<td>NELMIN = 6</td>
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<tr>
<td>EDIFF = 1E-07</td>
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<tr>
<td>ALGO = Normal</td>
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<td>LREAL = .FALSE.</td>
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</table>

<table>
<thead>
<tr>
<th># Ionic relaxation</th>
</tr>
</thead>
<tbody>
<tr>
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<td>IBRION = 2</td>
</tr>
<tr>
<td>ISIF = 3</td>
</tr>
<tr>
<td>ISYM = 2</td>
</tr>
<tr>
<td>EDIFFG = -0.001</td>
</tr>
<tr>
<td>ISMEAR = -5 or 0</td>
</tr>
<tr>
<td>SIGMA = 0.02</td>
</tr>
</tbody>
</table>

| Width of the smearing in eV. |

| SIGMA = 0.02 | Width of the smearing in eV. |
For the band structure calculation step, only the modified settings are shown in Table A-2. Other flags remain the same as in Table A-1. To incorporate the +U correction in the standard DFT model, the setting list in Table A-3 needs to be added to both Table A-1 and A-2. To execute the HSE calculation, the hybrid functional settings in Table A-4 needs to be added to both Table A-1 and A-2. Table A-4 also specifies the list of flags that need to be modified.

### Table A-2. List of the modified settings in the INCAR file for the band structure calculation step in the standard DFT model.

<table>
<thead>
<tr>
<th>Band Structure Calculation Step</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>ISTART = 1</td>
<td>Start the job using the pre-exist WAVECAR file.</td>
</tr>
<tr>
<td>ICHARG = 11</td>
<td>Keep the charge density constant to obtain eigen-values.</td>
</tr>
<tr>
<td>NSW = 0</td>
<td>No ionic relaxation.</td>
</tr>
<tr>
<td>IBRION = -1</td>
<td>No ionic relaxation.</td>
</tr>
<tr>
<td>ISYM = 0</td>
<td>No symmetry.</td>
</tr>
</tbody>
</table>

### Table A-3. List of INCAR flags that defines the +U correction in this work.

<table>
<thead>
<tr>
<th>LDA+U Method</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>LMAXMIC = 4</td>
<td>Effective on the d-orbital</td>
</tr>
<tr>
<td>LDAU = .TRUE.</td>
<td>Switches on the LDA+U method.</td>
</tr>
<tr>
<td>LDAUTYPE = 2</td>
<td>Specifies the type of LDA+U method.</td>
</tr>
<tr>
<td>LDAUU = 3.8</td>
<td>Effective on-site Coulomb interaction parameter.</td>
</tr>
<tr>
<td>LDAUJJ = 0.54</td>
<td>Effective on-site Exchange interaction parameter.</td>
</tr>
</tbody>
</table>

### Table A-4. List of INCAR flags that defines the HSE calculation in this work.

<table>
<thead>
<tr>
<th>HSE Method</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>LHFCALC = .TRUE.</td>
<td>Switches on the HF type calculations.</td>
</tr>
<tr>
<td>HFSCREEN = 0.2</td>
<td>Specifies where to truncate the long range Fock potential.</td>
</tr>
<tr>
<td>AEXX = 0.31</td>
<td>Fraction of exact Exchange potential</td>
</tr>
<tr>
<td>AGGAX = 0.69</td>
<td>Fraction of gradient correction to Exchange potential.</td>
</tr>
<tr>
<td>ALDAC = 1</td>
<td>Fraction of LDA Correlation potential</td>
</tr>
<tr>
<td>AGGAC = 1</td>
<td>Fraction of gradient correction of Correlation potential.</td>
</tr>
<tr>
<td>TIME = 0.4</td>
<td>The time step.</td>
</tr>
<tr>
<td>NKRED = 2</td>
<td>The k-space integral grid reduction factor.</td>
</tr>
</tbody>
</table>

# Modified settings in Table A-1

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>ISTART = 1</td>
<td>Start the job using the pre-exist WAVECAR file.</td>
</tr>
<tr>
<td>EDIFF = 1E-4</td>
<td>(also modify this flag in Table A-2)</td>
</tr>
<tr>
<td>IBRION = 1</td>
<td>Uses a simple charge mixer</td>
</tr>
<tr>
<td>ISYM = 3</td>
<td>Only the stress tensor and force are made symmetry.</td>
</tr>
</tbody>
</table>
APPENDIX B
POSCAR FILES

Figure B-1 shows the POSCAR file for the 4-atom GaN unit cell structure. It contains 2 Ga atoms and 2 N atoms. The “T” specifies which basis coordinate of the ions are allowed to move.

```
GaN:
  0.834227116959
  1.91135000 -3.31055531 0.00000000
  1.91135000 3.31055531 0.00000000
  0.00000000 0.00000000 6.26070000
  2 2
  Selective dynamics
  Direct
  0.33333333 0.66666667 0.00000000  T T T
  0.66666667 0.33333333 0.50000000  T T T
  0.33333333 0.66666667 0.37480000  T T T
  0.66666667 0.33333333 -0.12520000  T T T
```

Figure B-1. The POSCAR file describing a 4-atom GaN unit cell.

Figure B-2 shows the POSCAR file for the 32-atom GaN supercell structure. It was constructed from a pre-relaxed 4-atom unit cell. In this way, a faster convergence may be achieved. This POSCAR file contains 16 GaN atoms and 16 N atoms.
Figure B-2. The POSCAR file describing a 32-atom GaN supercell.
APPENDIX C
KPOINTS FILES

Figure C-1A and B show the k-mesh setups for the SC calculation of the unit cell and supercell structures, respectively.

\[
\begin{array}{c|cc}
\text{GaN: 4-atom} & \text{GaN: 32-atom} \\
\hline
\text{0} & \text{0} \\
\text{Gamma Monkhorst pack} & \text{Gamma Monkhorst pack} \\
\text{6} & \text{1} \\
\text{6} & \text{1} \\
\text{4} & \text{1} \\
\text{0.000} & \text{0.000} \\
\text{0.000} & \text{0.000} \\
\text{0.000} & \text{0.000} \\
\end{array}
\]

A

B

Figure C-1. The KPOINTS files used in the SC calculation step. A) A 4-atom unit cell, and B) a 32-atom supercell.

Figure C-2 shows the KPOINT files that specified a calculation along the \( \text{M-} \Gamma \) direction. The band structure along other high symmetric directions can be obtained by modifying the starting and ending nodes.

\[
\begin{array}{c|cc}
k-points along high symmetry lines \\
20 ! 20 intersections \\
\text{Line-mode} \\
\text{Reciprocal lattice} \\
0.000 0.500 0.000 ! \text{M} \\
0.000 0.000 0.000 ! \text{Gamma} \\
\end{array}
\]

Figure C-2. The KPOINT files used in the non-SC band structure calculation step.
LIST OF REFERENCES


Min Chu was born in Guangdong Province of China in October 1982. In 2005, she received her Bachelor of Science in electrical engineering from University of Science and Technology of China. She received her Master of Science in 2007 and Doctor of Philosophy in 2011 in the Computer and Electrical Engineering department at the University of Florida. Her Ph.D. research focused on the impact of strain on piezoresistive properties and reliability of novel device materials and structures.