Improving Transport Properties of GaN-Based HEMT on Si (111) by Controlling SiH\textsubscript{4} Flow Rate of the SiN\textsubscript{x} Nano-Mask

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Abstract: The AlGaN/AlN/GaN high electron mobility transistor structures were grown on a Si (111) substrate by metalorganic chemical vapor deposition in combination with the insertion of a SiN\textsubscript{x} nano-mask into the low-temperature GaN buffer layer. Herein, the impact of SiH\textsubscript{4} flow rate on two-dimensional electron gas (2DEG) properties was comprehensively investigated, where an increase in SiH\textsubscript{4} flow rate resulted in a decrease in edge-type threading dislocation density during coalescence process and an improvement of 2DEG electronic properties. The study also reveals that controlling the SiH\textsubscript{4} flow rate of the SiN\textsubscript{x} nano-mask grown at low temperatures in a short time is an effective strategy to overcome the surface desorption issue that causes surface roughness degradation. The highest electron mobility of 1970 cm\textsuperscript{2}/V·s and sheet carrier concentration of 6.42 × 10\textsuperscript{12} cm\textsuperscript{−2} can be achieved via an optimized SiH\textsubscript{4} flow rate of 50 sccm.

Keywords: GaN HEMT; SiN\textsubscript{x} nano-mask; edge threading dislocation; V-defects; 2DEG

1. Introduction

GaN-based high electron mobility transistors (HEMTs) have attracted much intense research because of its high-voltage operation, high-frequency switching, and high thermal conductivity for high-power and high-frequency device applications [1–3]. However, the growth of GaN-based HEMTs faces the problem of non-commercial nitride substrates, where sapphire (Al\textsubscript{2}O\textsubscript{3}) and silicon carbide (SiC) are two commonly used substrates. In recent years, to realize a compromise between high performance and wafer-size scalability, low cost, and integrated compatibility with the conventional Si-based technology, many research groups have grown GaN-based HEMT on a Si (111) substrate. Even so, the large lattice mismatch of 17% along with a thermal expansion coefficient mismatch of 54% between the Si (111) substrate and GaN layer is the most challenging of any epitaxial growth methods to achieve high-quality GaN layers. High-density dislocation (∼10\textsuperscript{10} cm\textsuperscript{−2}) and surface cracks due to thermal expansion during the cooling process are generally observed in the GaN/Si (111) layers, contributing to the degradation of the GaN-based HEMT performance. In general, the mainstream of research has focused on reducing the current collapse, which is attributed to both the interface trapping of AlGaN barrier/passivation layers and the bulk trapping of defects/dislocations [4–10]. To mitigate the bulk crystalline defects/dislocations, several buffer structural designs have been employed such as the graded/stepped AlGaN layer configurations [11–13], AlN/GaN or AlGaN/GaN superlattices (SL) [14–16], epitaxial lateral overgrowth (ELOG) technique [17], and the three-dimensional (3D)-to-two-dimensional (2D) growth mode [18,19]. Especially, inserting a SiN\textsubscript{x} nano-mask into the matrix of GaN layer to promote the growth mode transition in...
GaN from 3D island-like overgrowth to 2D coalescence has been becoming a widely used technique [19–33], in which the threading dislocations (TDs) are efficiently bent or even annihilate each other. There are several approaches to investigate the effect of SiNₓ nano-masks on the TD reduction such as varying either the SiNₓ deposition temperature or time to modulate the SiNₓ nano-mask configuration [19–22], using different growth conditions of the (Al)GaN layer overgrown on the SiNₓ nano-mask [23–25], or inserting multi-SiNₓ nano-mask into the (Al)GaN buffer layers [26–28]. Among these approaches, configuring a single SiNₓ nano-mask is considered the simplest strategy. By adjusting the growth time and temperature, the grain size and distribution of the SiNₓ nano-mask are modulated in such a way that the 3D-to-2D growth mode transformation is promoted [20,32]. However, any excess of the growth temperature and growth time will enhance the surface desorption of the GaN underlayer, leading to the aggregation of Ga atoms [33]. As a result, the threading dislocation density (TDD), etch pit density (EPD), and surface roughness of the GaN layers would increase, causing detrimental effects on the HEMT device performance. On the other hand, if the SiNₓ nano-mask is grown at too low temperature or short duration, its grain size would be tiny and ineffective to generate the transition of 3D-to-2D growth mode as well as to suppress the TDD. It is therefore essential to study an alternative method to solve the surface desorption issue, while retaining the efficiency of the inserted-SiNₓ nano-mask, in terms of suppressing TDs and improving two-dimensional electron gas (2DEG) properties of the GaN HEMT structure.

For this conversation, we present inserting a SiNₓ nano-mask into the low-temperature GaN (LT-GaN) layer grown by metalorganic chemical vapor deposition (MOCVD), where the nano-mask formation was controlled via the SiH₄ flow rate variation instead of either the growth temperature or the growth time. Thus, this novel method allows easily controlling the SiNₓ configuration, enhancing the annihilation of TDs. Importantly, its low temperature and short-time growth were expected to highly limit the surface desorption of GaN underlayer. The results in this study show that the crystalline quality and the transport properties of GaN-based HEMT structure were strongly governed by varying the SiH₄ flow rate.

2. Experimental

The full structures of GaN-based HEMT were grown on 6" Si (111) substrates by the G4 MOCVD system (Aixtron, Herzogenrath, Germany). The conventional precursors including TMGa, TMAl, NH₃, and silane (1% diluted-SiH₄) were used for the Ga, Al, N, and Si source, respectively. In order to grow the lattice-matched GaN layer on the Si (111) substrate, an AlN nucleation layer of about 300 nm was initially grown to prevent Ga–Si melt-back etching, followed by a transition layer of ~1.8 µm. This is to effectively modulate stress and prevent misalignment. A semi-insulating LT-GaN buffer layer with a thickness of 1.8 µm was then deposited at 990 °C, followed by a 2DEG heterostructure. This 2DEG structure was composed of a 300 nm HT-GaN (1020 °C) channel layer, 0.5 nm AlN spacer layer, and 10 nm Al₀.₂₅Ga₀.₇₅N barrier layer as shown in Figure 1. Finally, the structure was capped by a 4 nm thin GaN layer to protect the wafer surface from oxidation. To study the effect of the SiNₓ nano-mask on reducing the stress and TDD, the SiNₓ nano-mask was inserted at 300 nm above the LT-GaN/transition layer interface as can be seen in Figure 1. The growth time of the nano-mask was 1 min, while the growth temperature and the ammonia gas flow were kept at the same with that of the LT-GaN layer. Herein, a highly concentrated 1%-SiH₄ source was employed to conduct a high deposition rate and low surface desorption. Five samples with different SiH₄ source flow rates of 0, 25, 50, 75, and 100 sccm were used and denoted as samples A, B, C, D, and E, respectively. Sample A is a control sample, where no SiNₓ nano-mask was inserted. The in situ reflectivity and curvature measurement were monitored simultaneously by the LayTec EpiCurve-TT (LayTec, Berlin, Germany) unit integrated inside the MOCVD chamber. The 633 nm light source and 650 nm laser beam were used for reflectivity and curvature characterization, respectively. The experimental etching pit density (EPD) was performed in molten-KOH
The in situ monitoring of the reflectivity and surface curvature of all five samples is shown in Figure 2. The growth rate and surface morphology of the samples during the epitaxial growth could be evaluated from the reflectivity measurement (Figure 2a). Before the SiN$_x$ nano-mask growth, the growth rate of ~4.2 µm/h of the 300 nm thick LT-GaN initial layer of all samples was indicated from the dependence of reflectance oscillation on the growth time. During the SiN$_x$ nano-mask insertion, the reflectance intensity of the samples was extinguished and flattened because of depositing 3D SiN$_x$ nanocrystals. Then, the maximum intensity of the oscillation peaks was gradually restored during the 1.5 µm LT-GaN overlayer growth, where the required time to recover the reflectance peak intensity to maximum, as before the SiN$_x$ deposition, was different between the inserted SiN$_x$ samples. Obviously, the recovering time, marked as the length of colored arrows in Figure 2a, increased with increasing the SiH$_4$ flow rate. In other words, the time required for the growth mode transition from 3D-island to 2D-coalescence of the LT-GaN overlayer strongly depends on the SiH$_4$ flux, in which transition time increases with the amount of SiH$_4$ flux used. It is also emphasized that this transition could not complete if the SiH$_4$ flow rate exceeds a threshold of 75 sccm, as in the case of sample E. Indeed, the reflectivity at the end of the LT-GaN overlayer of this sample only equals ~40% as compared to that at
end of the LT-GaN underlayer. However, the following high-temperature GaN (HT-GaN) channel layer growth of this sample exhibited a fast restoration in the reflectivity only after three oscillation cycles (see blue-dash arrow in Figure 2a, sample E). This result suggests that the SiH\textsubscript{4} flux modulation during inserting SiNx interlayer is a considerable approach in terms of recovering the 2D growth mode of the HT-GaN layer even if a SiH\textsubscript{4} flux as high as 100 sccm is used.

![Figure 2. In situ (a) reflectivity and (b) curvature monitoring of sample surfaces.](image)

To study the surface morphology with varying SiH\textsubscript{4} flow rate, scanning electron microscopy (SEM) and atomic force microscopy (AFM) were employed as shown in Figure 3a–j. No V-defects were observed on the surfaces of samples B and C, while a few defects were visible on both sample D and sample E. The SEM image (Figure 3d) of sample D exposes several small pits. These pits are well known as stacking mismatch boundary (SMB) defects, attributed to the atom alignment faults during the coalescence process. Meanwhile, the surface of sample E displays the additional appearance of hexagonal micro-pit (HMP) defects, which are caused by the incomplete coalescence process as mentioned in the reflectivity discussion (Figure 2a) [34]. The presence of SMB and HMP defects on these samples is expected to decline the transport properties of 2DEG, which is discussed later. On the other hand, the surface morphologies of the inserted SiNx samples were preserved as the control sample with a root mean square (RMS) roughness of around 0.22 nm as shown in
Figure 3f–j. This result indicates clearly that the surface desorption of LT-GaN underlayer in our study was restrained efficiently during SiNₓ interlayer growth.

Figure 3. (a–e) SEM and (f–j) AFM images of the inserted SiNₓ nano-mask samples with various SiH₄ flow rates.

Figure 2b shows that all five samples were suffering compressive strains, where the strain in the transition layer and 300 nm LT-GaN underlayer increased slowly with the growth time. After inserting the SiNₓ nano-mask, the compressive strain in the LT-GaN overlayer of the SiNₓ samples (samples B–D) increased in the same fashion, quickly approaching the strain magnitude of sample A. This is in agreement with the reflectivity results, where a transition from 3D island-like to 2D growth mode in the following LT-GaN layers was taking place. Furthermore, note that the strain increasing rate of sample E was much lower than that of other samples as can be seen in Figure 2b. Thus, the compressive strain of sample E (highest SiH₄ flow rate of 100 sccm) was relieved more effectively than in other samples. That is because the transformation from 3D to 2D growth mode of the LT-GaN overlayer is not completed in this sample, as the reflectivity results indicated (Figure 2a). Indeed, it is directly related to the morphology as revealed by SEM (Figure 3e), where the long 3D growth mode duration of the LT-GaN overlayer and the incomplete coalescence of the HT-GaN channel layer resulted in the formation of HMP defects. Moreover, measurements of curvature showed that strain of layers is strongly affected by SiH₄ flow rate that is also in agreement with the ex situ wafer bow measurements, in which the positive warp of sample A, B, C, D, and E were 22.0, 15.7, 15.7, 14.8, and 9.6 µm, respectively. Obviously, the warp of 9.6 µm presented in sample E is much smaller than that of other samples.

In order to investigate the relationship between the TDD and the SiH₄ flow rate, the EPD and X-ray diffraction (XRD) techniques were employed, and the results are summarized in Table 1. The omega XRD scan of the sample near (002) and (102) plane could be found in Figure S1. The EPD slightly decreased as the SiH₄ flow rate was increased from 25 to 75 sccm. However, it rapidly reduced to $3.24 \times 10^8$ cm⁻² when the SiH₄ flow rate increased further to 100 sccm (sample E). Of course, the EPD directly relates to the TDD in the epilayers. Herein, the TD in GaN growth could be categorized into two types as screw-type TD and edge-type TD. The TDD of each type presented in the GaN layer can be identified from the FWHM of (002) and (102) X-ray rocking curves (i.e., $\beta_{(002)}$ and $\beta_{(102)}$) via the following formulas [11].

\[
D_{\text{screw}} = \frac{\beta_{(002)}^2}{4.35 \times b_{\text{screw}}} \\
D_{\text{edge}} = \frac{\beta_{(102)}^2 - \beta_{(002)}^2}{4.35 \times b_{\text{edge}}}
\]
Table 1. Dependence of dislocation density on the SiH₄ flow rate by XRD and EPD analysis.

| Sample ID | SiH₄ Source (sccm) | FWHM (arcsec) | TDD (cm⁻²) | EPD (cm⁻²) | Wafer Bowing (μm) |
|-----------|--------------------|---------------|------------|------------|------------------|
|           |                    | (002)         | (102)      | Screw-Type | Edge-Type        |
| A         | 0                  | 46 ± 65       | 945 ± 5    | (4.36 ± 0.09) × 10⁸ | (3.59 ± 0.02) × 10⁹ | 6.52 × 10⁸ | 22.0 |
| B         | 25                 | 468 ± 5       | 920 ± 5    | (4.40 ± 0.09) × 10⁸ | (3.33 ± 0.02) × 10⁹ | 5.76 × 10⁸ | 15.7 |
| C         | 50                 | 466 ± 5       | 908 ± 5    | (4.36 ± 0.09) × 10⁸ | (3.23 ± 0.02) × 10⁹ | 5.52 × 10⁸ | 15.7 |
| D         | 75                 | 467 ± 5       | 872 ± 5    | (4.38 ± 0.09) × 10⁸ | (2.88 ± 0.02) × 10⁹ | 5.34 × 10⁸ | 14.8 |
| E         | 100                | 441 ± 5       | 786 ± 5    | (3.91 ± 0.09) × 10⁸ | (2.25 ± 0.02) × 10⁹ | 3.24 × 10⁸ | 9.6  |

The screw-type TDD ($D_{screw}$) and edge-type TDD ($D_{edge}$) are computed from $\beta_{(002)}$, $\beta_{(102)}$, and burger vector length ($b_{screw} = 0.5185$ nm and $b_{edge} = 0.3189$ nm). The extracted TDDs of all samples are displayed in Table 1. Interestingly, the edge-type TDD decreased considerably with the increasing SiH₄ flow rate, whereas the screw-type TDD showed a slight drop as SiH₄ flow is more than 75 sccm. Thus, the increasing SiH₄ flow rate during SiNx nano-mask forming has a dominant effect on the decrease in edge-type TDD rather than screw-type TDD. We notice that this result plays an important role in improving the 2DEG properties of the AlGaN/GaN HEMT structure.

To further understand the mechanisms of the decreasing edge-type TDD, the cross-sectional bright-field scanning transmission electron microscopy (STEM) micrograph of sample E was taken as can be seen in Figure 4. The edge dislocations, screw dislocations, and mixed dislocations (edge and screw dislocations) are labeled as E, S, and M, respectively. By the comparison between two STEM images observed along $g = [0002]$ and $g = [TT20]$ zone axis, the edge dislocation density is distinctly reduced. Apparently, the propagation of most of TDs was terminated or bent at the SiNx interlayer and further annihilated during the 2D lateral overgrowth on 3D island-like LT-GaN overlayer, which is marked as white-dash lines in Figure 4. Three kinds of interaction between edge-type TDs are visible: (1) Type I is parallel, two TDs passed through the SiNx nano-mask with the same Burgers vector; (2) Type II is fusion, two TDs combined to form a new TD where its Burgers vector equals to the sum of two componental Burgers vectors. (3) Type III is annihilation, two TDs with the opposite Burgers vectors react against each other [33,35]. We notice that only type II and III interactions benefit the annihilation of TDs.

Figure 4. (a) Bright-field cross-sectional STEM micrograph of GaN-based HEMT structure on Si (111) with the SiNx nano-mask grown under 100 sccm SiH₄ flow rate and (b) Selective area electron diffraction pattern of the HT-GaN top layer taken along the [1100] zone axis.
The effect of the SiH$_4$ flow rate on the transport properties of 2DEG HEMT structures was carried out by van der Pauw–Hall measurements at room temperature (RT) and the results are shown in Figure 5. Below a SiH$_4$ flow rate of 50 sccm, both the mobility and the sheet carrier concentration ($N_S$) of 2DEG structure enhanced simultaneously with increasing the SiH$_4$ flow rate. This behavior could be explained by the decrease in the edge-type TDs in the structure as observed from XRD results [32,36]. The edge-type TDs are usually accompanied by the dangling bonds. These dangling bonds generate an acceptor-like trap level in the band structure, capturing free charges and then forming negatively charged Coulombic scattering centers. Thus, any reduction in edge-type TDD is related to an improvement of the 2DEG mobility [37]. Meanwhile, the $N_S$ was also influenced by the edge-type TDD. The increase of $N_S$ with decreasing edge-type TDs is a result of the restrained charges at the acceptor-like traps [36,38]. As the SiH$_4$ flow rate was increased further to 75 sccm (sample D), both the mobility and $N_S$ significantly degraded. It could be due to the formation of the nonuniform distribution of SMB defects as can be seen in Figure 3d. The appearance of SMB defects reflects the interface roughness and electrical field fluctuation at the 2DEG structure, leading to a decrease in mobility and $N_S$ [39–41]. A further decrease in 2DEG mobility of sample E is understandable, ascribed to the formation of not only SMB but also HMP defects as can be observed in Figure 3e. Interestingly, the $N_S$ of this sample increased as compared to sample D. This may be explained by the active diffusion of Si adatoms from the SiN$_x$ nanostructures. Under a SiH$_4$ flow rate as high as 100 sccm, the excess Si adatoms from the SiN$_x$ nano-mask could diffuse and precipitate on the sidewalls of the HMP defects via the TDs [26,33]. In addition, we notice that this diffusion process could be even boosted under a 3D growth mode of GaN channel layer as observed in our case (see sample E in Figure 2a). The Si adatoms preferentially sticking on the sidewalls of the HMP defects play a role as donors and releases electrons to the GaN channel layer. As a result, it causes an increase in the $N_S$ of the 2DEG structure. Besides that, the Si diffusion and incorporation into TDs could be a pathway causing unexpected leakage currents. Similarly, this effect was also observed in the Mg-doped GaN film. The segregated Mg propagates through TDs and incorporates at the boundaries of pyramidal inversion domains (PIDs) to form an Mg-rich area, degrading device performance [42–44].

Figure 5. (a) Mobility and NS of the 2DEG structure as a function of the SiH$_4$ flow rate. The inset (b) shows the dependence of sheet resistance ($R_S$) on the SiH$_4$ flow rate.
4. Conclusions

In conclusion, the fabrication of AlGaN/AlN/GaN HEMT structures with high mobility and $N_S$ has been demonstrated via modulating the SiH$_4$ flow rate of the SiN$_x$ nano-mask. The surface roughness of the samples was maintained at 0.22 nm, proving an effective elimination of surface desorption issue from the LT-GaN underlayer during inserting the SiN$_x$ nano-mask. More importantly, the SiN$_x$ nano-mask effectively contributed stress relaxation via promoting 3D-to-2D growth mode transformation of the LT-GaN overlayer and bending or annihilating TDs. Thus, it helped to reduce the edge-type TDD and EPD of the GaN-based HEMT structure as low as $2.25 \times 10^6$ and $3.24 \times 10^6$ cm$^{-2}$, respectively, as observed in the sample grown using 100 sccm SiH$_4$ flow rate. However, when the SiH$_4$ flow rate was larger than 50 sccm, an oversized SiN$_x$ nano-mask could be presented, resulting in the development of V-defects as SMB and HMP defects. These defects would be located at or near the 2DEG structure, causing degradation of the 2DEG mobility and sheet carrier concentration. Consequently, the highest mobility and $N_S$ of the sample can be achieved to be $-1970$ cm$^2$/V·s and $6.42 \times 10^{12}$ cm$^{-2}$, respectively, under an optimized SiH$_4$ flow rate of 50 sccm. Interestingly, the $N_S$ of sample E exhibited a reverse trend, which may be attributed to the accumulation of the diffused Si adatoms from the SiN$_x$ nano-mask on the sidewalls of HMP defects as the SiH$_4$ flux was used as high as 100 sccm.

Supplementary Materials: The following are available online at https://www.mdpi.com/2079-6412/11/1/16/s1, Figure S1: Normalized XRD rocking curves of GaN, (a) (002) and (b) (102) planes. (c) FWHM as a function of SiH$_4$ flow rate of (002) and (102) planes.

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