Effect of defects on strain state in nonpolar \(a\)-plane GaN

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We have investigated the influence of basal stacking fault (BSF) and impurity related defect on the strain state of \(a\)-plane GaN epilayers. Four \(a\)-plane GaN epilayers were grown on \(r\)-plane sapphire using different growth strategies by metalorganic chemical vapor deposition. It is found that with a growing number of stacking fault, both the anisotropic in-plane strain and compressive out-plane strain along \(c\)-axis are relieved. Epitaxial lateral overgrowth with a TiN interlayer is an effective way to relieve in-plane strain and reduce BSF density. The extrapolated lattice parameters free of biaxial strain increase with the normalized yellow luminescence intensity. Hydrostatic strain induced by impurity-related defects is the possible cause of this phenomenon.

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1. Introduction

Group III Nitrides are suitable to fabricate both optoelectronic and electronic devices \([1]\). The most commonly used devices are fabricated on \(c\)-plane sapphire substrate, because it is easy to achieve desirable crystalline quality and smooth surface on that plane \([2]\). However, the strong piezoelectric field in \(c\)-plane as-grown III Nitride heterostructure is detrimental to the performance of optical devices due to so-called quantum-confined Stark effect \([3]\). Therefore, the nonpolar and semipolar III nitrides are proposed to address this issue \([4,5]\). Light emitting diodes (LEDs) and laser diodes (LDs) based on nonpolar and semipolar GaN have demonstrated a better performance in some wavelengths than conventional one on the \(c\)-plane, and with less peak shift due to current increase \([6,7]\). One the other hand, this piezoelectric field produces high density two dimensional electron gas, which may cause trouble in enhancement-mode AlGaN/GaN field-effect transistors process. This obstacle can also be overcome using nonpolar AlGaN/GaN heterostructures \([8]\).

The strain in \(a\)-plane GaN layer is anisotropic, which may introduce anisotropic optical and electrical properties and influence device’s performance \([9,10]\). The number of available reciprocal lattice points for \(a\)-plane GaN is limited due to its geometry in diffraction measurements. So the precise determination of lattice parameter of nonpolar epilayers is somewhat complicated. A few methods have been reported, either by measuring several symmetric and skew-symmetric planes at multiple azimuth positions in an edge-symmetric geometry \([11]\), or by calculating interplanar spacings from a combination of symmetric, asymmetric, and skew-symmetric reflections \([12,13]\). BSFs, together with partial dislocations (PDs), are the main defects in non-polar GaN layers \([14]\). The influence of undesirable relaxation, caused by BSFs origination, on InGaN quantum wells grown on \(m\)-plane GaN has been reported \([15]\), and anisotropic strain relaxation in nonpolar GaN has been attributed to the formation of SFs \([16]\). However, detailed relationship between strain state and defects is not well understood.

In this work, four different nonpolar GaN samples were analyzed by high resolution X-ray diffraction (HRXRD). Lattice parameters were determined using the method proposed by Laskar et al. \([13]\), and BSF densities were determined by TEM, and the method proposed by Moram et al. \([17]\). The relationship between BSF density and strain state was found and discussed. Simultaneously, we extrapolated the lattice parameters free of biaxial strain. Room temperature photoluminescence (PL) was used to estimate impurity related defect. The correlation between normalized yellow luminescence (YL) intensity and hydrostatic strain was analyzed.

2. Experimental procedure

Nonpolar \(a\)-plane GaN epilayers were grown on \(r\)-plane sapphire substrate by metalorganic chemical vapor deposition (MOCVD). A series of samples with different scales of BSFs and dislocations were obtained by various growth strategies.
The lattice parameters, as well as distortion angle, were measured for each sample. For the limitation of intensity, some reflections were not measured for samples with inferior crystal quality. The least square method proposed by Laskar was adopted to minimize the error in measurement. HRXRD measurement was carried out to determine lattice parameters standing for BSF density using a Bruker D8 Discover HRXRD equipped with a Ge (220) four bounce monochromator crystal. The direct precision measurement of scattering angle method suggested by Fewster was adopted to minimize the error in measurement [20]. PL measurement was conducted to figure out the impurity related defect density using a 325 nm He–Cd laser.

### 3. Results and discussion

The epitaxial relationship of a-plane GaN film on r-plane sapphire is: [0001] GaN || [11-20] sapphire, [–1100] GaN || [11–20] sapphire [5]. The lattice mismatch and thermal expansion mismatch between GaN and sapphire are different along the two main in-plane directions. Therefore, there is an anisotropic strain and the hexagonal unit cell is distorted [9]. The schematic diagram of such a distorted wurtzite unit cell is shown in Fig. 2, where the physical meanings of different lattice parameters are also given. At least three lattice parameters are needed to fully understand the unit cell: a_s (sidewall), a_t (top), and c. To calculate the lattice parameters, 2θ-values of up to nine reflections were measured for each sample (for the limitation of intensity, some reflections were not measured for samples with inferior crystalline quality), in symmetric, skew symmetric or asymmetric geometry. Using the least square method proposed by Laskar et al. [13], the lattice parameters as well as distortion angle δ were obtained. The measured 2θ-values are shown in Table 1, and the calculated lattice parameters are listed in Table 2. Although X-ray probing depth varies among different reflections, all GaN epilayers under study are penetrated by X-ray in all geometries, except sample D, which has a relatively thicker re-grown GaN layer.

It has been suggested that compared to (30–30) reflection, in which BSFs are invisible, both (10–10) and (20–20) reflections can be influenced by BSF density [17]. Rocking curves of (20–20) shown in Fig. 3 were measured with an open detector. By measuring the intensity of a specific point arbitrary distance (say, 0.8°) away from the peak of (20–20) rocking curve, i.e. the intensity of diffusion scattering caused by BSF, one can estimate the BSF density. Therefore, BSF density declines monotonically from sample A to sample D.

### Table 1

<table>
<thead>
<tr>
<th>Plane of reflection</th>
<th>Measured 2θ_{hkl} (deg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>B</td>
</tr>
<tr>
<td>(11–20)</td>
<td>57.756</td>
</tr>
<tr>
<td>(10–10)</td>
<td>32.381</td>
</tr>
<tr>
<td>(21–30)</td>
<td>–</td>
</tr>
<tr>
<td>(2–1–10)</td>
<td>–</td>
</tr>
<tr>
<td>(11–22)</td>
<td>69.139</td>
</tr>
<tr>
<td>(10–11)</td>
<td>36.841</td>
</tr>
<tr>
<td>(10–12)</td>
<td>–</td>
</tr>
<tr>
<td>(21–31)</td>
<td>97.663</td>
</tr>
<tr>
<td>(21–32)</td>
<td>–</td>
</tr>
</tbody>
</table>

### Table 2

<table>
<thead>
<tr>
<th>Lattice parameters</th>
<th>Calculated values</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>A</td>
</tr>
<tr>
<td>c (Å)</td>
<td>5.1758</td>
</tr>
<tr>
<td>a_s (Å)</td>
<td>3.1909</td>
</tr>
<tr>
<td>a_t (Å)</td>
<td>3.1895</td>
</tr>
<tr>
<td>δ (deg)</td>
<td>–0.03</td>
</tr>
</tbody>
</table>
images, which are not shown here), the PD density follows the
same trend as BSF. Obviously, diffusion scattering intensity in
XRD (200) rocking curve is proportional to TEM BSF result. Thus it
provides a sound method in this case to estimate BSF density in a
fast and nondestructive way.

The x, y and z axes are chosen along GaN [11–20], [−1100],
[0001] directions, respectively. Strains in respective directions are
calculated by the equation
\[ e_{xx} = \frac{(a_x - a_0)}{a_0}, \]
\[ e_{yy} = \frac{(a_y - \sqrt{3}a_0)}{\sqrt{3}a_0}, \]
\[ e_{zz} = \frac{(c - c_0)}{c_0}, \]
where \( a_x = a_s \) and \( a_y = 2a_t \sin(60 - \delta/2), \)

denoting lattice parameters along x and y axis, respectively. The
ideal lattice parameters chosen for GaN are \( a_0 = 3.1896 \text{ nm} \) and
\( c_0 = 5.1855 \text{ nm} \) [21]. Assuming a zero \( \sigma_{xx} \) along [11–20] direction
(a biaxial strain), and using \( e_{xx} \) and \( e_{zz} \) determined by XRD, strain
component in y-axis can be calculated theoretically by the
following equation:
\[ e_{yy} = \frac{C_{11}}{C_{12}} e_{xx} - \frac{C_{13}}{C_{12}} e_{zz}, \]
where \( C_{11}, C_{12} \) and \( C_{13} \) are stiffness constants for GaN, and the
values from Ref. [22] are adopted. The experimentally determined
and theoretically calculated value \( e_{yy} \) agree fairly well, which
proves the method using here is reliable. The existing
discrepancies between them are caused by errors in measurement,
and the inaccuracy of stiffness constant. Also, it could be
partly attribute to the deviation of the assumption of biaxial
strain, which would be discussed later.

In Fig. 5, the strains (experimental) are plotted versus BSF
density determined by TEM. Along direction perpendicular to
surface, samples are nearly fully relaxed or in tensile strain, while
in basal plane layers are compressed, both are consistent with
theoretical prediction and experiment conducted by other
researchers [9]. It is obvious that with an increasing BSF density,
the in-plane distortion is eased. However, sample D, whose BSF
density is the smallest, is significantly relaxed in basal plane
compared to sample C. There are four different types of BSF in
\( a \)-plane GaN, I1, I2, I3 and E, the former three are intrinsic and the
last extrinsic. I1 type has the lowest formation energy, I3 and I2
have the second- and third-lowest, while that of E is even higher.
Prismatic stacking faults (PSFs), another kind of SF, also has a high

![Fig. 3. Open detector rocking curves of (20−20) reflection. The specific points −0.8’ away from the peak are marked in the picture.](image)

![Fig. 4. Bright filed TEM images of plan-view samples (g = 1–100). (a)-(d) correspond to sample A–D, respectively.](image)
formation energy (60 times higher than that of $l_1$ type BSF), thus has a significantly low density (about $10^7$ cm$^{-2}$) [16,23]. Therefore, $l_1$ type BSF is the dominate SF in nonpolar epilayers. $l_1$ type BSF can be bounded by a sessile Frank–Shockley dislocation with Burgers vector $b=1/6\langle 2 \ 203 \rangle$, while $l_2$ type BSF can be formed by $1/3\langle 1 \ -100 \rangle$ shear of one part of a crystal with respect to the other or by dissociation of a perfect dislocation $b=1/3\langle 11 \ -20 \rangle$ into two Shockley partials with $b=1/3\langle 1 \ -100 \rangle$ [14]. All have a weight along $y$-axis in basal plane, so they are able to relieve the anisotropic compression along $y$-axis. As an epitaxial lateral overgrowth (ELOG) method on TiN porous template was used, sample D does not follow this trend, which should be attribute to the change of strain state in re-growth process. In ELOG process, the so called wing areas are lateral grown on the mask, thus they are less influenced by misfit (both lattice misfit and thermal expansion misfit) between re-growth layer and substrate. It has been pointed out that the wing areas in conventional ELOG on stripe shape mask are almost free of strain based on microscroscopy CL analysis [23]. Therefore, it can be concluded ELOG using TiN interlayer can also achieve similar result.

Another interesting phenomenon is the different strain states between B and D. For all samples, GaN are compressed along $c$-axis, irrespective of the variation of in-plane strain and BSF densities. Though with the same strain in basal plane, sample B is less strained along $c$-axis than sample D. BSF density is much higher in sample B than D. $l_1$ type BSFs can be seen as a removal of basal plane or insertion of basal plane, and bounded by PDs with burgers vector $1/6\langle 2 \ 203 \rangle$. Therefore, with its non-zero weight along $z$-axis, $l_1$ type BSF is also effective to relax the strain in this axis. It should be noted that because sample A and B suffer from lacking effective crystal planes in measurement, the lattice parameter error, especially for that along in-plane directions, is relative large. The irregular variation from sample A to C is partly caused by this issue. Besides, the influence of hydrostatic strain, which will be discussed in the latter part, should not be neglected in sample B.

In order to demonstrate other possible causes to this strain state variation, the effect of biaxial stress and hydrostatic stress strain should be separated, so the lattice parameter free of biaxial strain (represented by $c_0'$ and $c_0''$) is desirable [24]. For $a$-plane GaN epilayers, adopting the ratio $c_0'/c_0=1.62575$ [21], Eq. (2), which is derived from Eq. (1), is used to extrapolate this kind of lattice parameters

$$\frac{c-c_0}{c_0} = \frac{C_{11}}{C_{13}} \left( \frac{d_1-1}{d_1} + \frac{d_3}{d_3} \right) = 0$$

where the physical meaning of $d_1$ and $d_3$ are displayed in Fig. 1, $d_{10}$ and $d_{20}$ are the value of $d_1$ and $d_3$ in undistorted unit cell, so $d_{10} = 2d_{100} = d_{10} a_c$, $d_{20} = d_{10} \sqrt{3} = \frac{1}{2} d_{100} a_c$. The calculated lattice parameters $c_0'$ are plotted in Fig. 6(b). It is obvious that the hydrostatic strain is much smaller than the total strain, thus it means the biaxial stress is dominate. There is no evidence showing that BSF density is relevant to hydrostatic strain.

In fact, the variation of hydrostatic strain is related to defects other than BSF. Yellow band around 2.2 eV in PL spectrum is an indicator of defect density, especially impurity related defect density [19,25]. The result of PL for the four samples is shown in Fig. 6(a), in which the intensities are normalized according to the main origin of yellow band [25,26], act as shallow donors and can introduce additional electrons [27]; so lattice parameter increases with the increase electron concentration [28]. Detailed analysis about what specific kinds of defect result in this change in hydrostatic strain is
beyond the scope of this work, but it indicates that the reduction of BSF is not necessarily along with that of other kinds of defects.

Sample D appears abnormal in Fig. 6(b). Because for a 325 nm excitation, the probing depth is 40 nm in GaN [29], thus only overgrown layer is probed in PL; while the X-ray can penetrate the whole GaN layer in some reflections, so the lattice parameter derived from XRD is a value including the influence of both template and overgrown GaN layer. In sample D, the lattice parameter of template GaN layer is believed larger than that of overgrown layer due to its higher defect incorporation and carrier concentration. Therefore, sample D shows a little larger lattice parameter free of biaxial strain than predicted.

4. Conclusions

In conclusion, the effect of defect on lattice parameter and strain state is studied. It is evident that with an increasing number of BSF, strain both in and out of basal plane can be relaxed. This kind of relaxation is caused by BSF related PDs, whose burgers vector have non-zero weights both in and out of basal plane. The adoption of a TiN micro-mask layer and sub-sequent ELOG can also significantly relax strain in all directions. Hydrostatic strain is secondary to biaxial strain, and lattice parameter free of biaxial strain increases with the normalized YL intensity, indicating that hydrostatic strain is closely related to impurity related defect, just as it does in c-plane case.

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