**Introduction**

Although Si-based electronics are used to power light-emitting diodes and electric vehicles, their utility in high power applications is limited by a low breakdown voltage. The most promising alternative power devices consist of vertical GaN devices, which often require regrown active regions. Here, we report on X-ray diffraction studies of the crystallinity of the GaN p-i-n structures prepared with and without ex-situ ambient exposure and/or chemical etching.

**GaN for High Power Electronics**

- Blue: LEDs and electric vehicles utilize silicon-based power electronics [1].
- Yellow: Power transmission and distribution require alternative approaches [1].

**Regrowth Interface at p-n Junction**

<table>
<thead>
<tr>
<th>GaN Substrate</th>
<th>In-situ Regrowth</th>
<th>Ex-situ Regrowth</th>
<th>ICP Regrowth</th>
</tr>
</thead>
<tbody>
<tr>
<td>2um UID GaN</td>
<td>3um UID GaN</td>
<td>2um UID GaN</td>
<td>3um UID GaN</td>
</tr>
<tr>
<td>300um n-GaN</td>
<td>300um n-GaN</td>
<td>300um n-GaN</td>
<td>300um n-GaN</td>
</tr>
</tbody>
</table>

**Symmetric and Asymmetric Scans**

**(0004)**

<table>
<thead>
<tr>
<th>Sample</th>
<th>(\theta_0) (arcsec)</th>
<th>(\eta) (from (\Delta\theta))</th>
<th>(a_\nu) (10^4 rad)</th>
<th>(b_\nu) ((\mu)m)</th>
<th>(\Delta\theta = \theta_0) (10^4 rad)</th>
<th>(N_\nu) (10^6 cm^-2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>In-situ</td>
<td>52</td>
<td>0.428</td>
<td>1.5</td>
<td>1.9</td>
<td>1.7</td>
<td>528</td>
</tr>
<tr>
<td>Ex-situ</td>
<td>68</td>
<td>0.033</td>
<td>3.2</td>
<td>8.6</td>
<td>11.1</td>
<td>454</td>
</tr>
<tr>
<td>ICP Etched</td>
<td>59</td>
<td>0.229</td>
<td>2.2</td>
<td>4.2</td>
<td>2.4</td>
<td>162</td>
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<tr>
<td>Substrate</td>
<td>50</td>
<td>0.222</td>
<td>1.9</td>
<td>3.1</td>
<td>3.0</td>
<td>108</td>
</tr>
</tbody>
</table>

**Threaded Dislocations (TDs)**

- Screw-type TDs
- Edge-type TDs

**How can we quantify screw- and edge-type dislocation densities?**

**High Resolution X-ray Diffraction (HRXRD)**

Bragg’s Law: \(\beta_\nu = 2\theta_\nu \sin \beta\)

**Pseudo-Voigt Analysis of HRXRD**

\[ L_\nu = \nu_0 \frac{(1+\nu_0) + (1-\nu_0)|x|}{(1+\nu_0) + (1-\nu_0)|x|} \]

\[ c(x) = \frac{c_0}{(1+\nu_0) + (1-\nu_0)|x|} \]

\[ \beta = \beta_\nu \frac{c(x)}{c(x)} \]

<table>
<thead>
<tr>
<th>Sample</th>
<th>(\beta_\nu) (arcsec)</th>
<th>(\eta) (from (\Delta\beta))</th>
<th>(a_\nu) (10^4 rad)</th>
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</thead>
<tbody>
<tr>
<td>ICP + TBCI</td>
<td>70</td>
<td>0.059</td>
<td>3.2</td>
<td>8.5</td>
<td>6.6</td>
<td>12.3</td>
</tr>
<tr>
<td>ICP + TBCI Regrowth</td>
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<td>0.267</td>
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<td>2.5</td>
<td>12.3</td>
</tr>
<tr>
<td>TBCI</td>
<td>37</td>
<td>0.372</td>
<td>1.2</td>
<td>1.1</td>
<td>2.6</td>
<td>12.3</td>
</tr>
<tr>
<td>TBCI Regrowth</td>
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<td>0.547</td>
<td>0.9</td>
<td>0.7</td>
<td>1.9</td>
<td>12.3</td>
</tr>
<tr>
<td>ICP</td>
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<td>2.9</td>
<td>12.3</td>
</tr>
<tr>
<td>ICP Regrowth</td>
<td>69</td>
<td>0.117</td>
<td>3.6</td>
<td>12.2</td>
<td>2.9</td>
<td>12.3</td>
</tr>
<tr>
<td>Substrate</td>
<td>48</td>
<td>0.201</td>
<td>1.0</td>
<td>3.0</td>
<td>3.3</td>
<td>12.3</td>
</tr>
</tbody>
</table>

**Probing the structure with XRD & RBS**

**Probing the structure using XRD:**
- **Ex-situ** and **ICP Etched** had the largest screw-type TD densities.
- In-situ had the lowest screw-type TD density and the highest edge-type TD density.

**Probing electronic properties using cathodoluminescence**
- Donor acceptor pair emission (DAP) near the surface is lowest for **Ex-situ** and **ICP Etched**.
- DAP emission at the regrowth interface is enhanced for **ICP etched**.

**Ambient air exposure worsens crystallinity and electronic properties, but ICP etching can partially restore the electronic properties.**

---

1. Materials Science and Engineering, 2Michigan Ion Beam Laboratory, University of Michigan, Ann Arbor, MI 48109, USA
2. Department of Electrical Engineering, Yale University, New Haven, CT 06520, USA
Introduction

Although Si-based electronics are used to power light-emitting diodes and electric vehicles, their utility in high power applications is limited by a low breakdown voltage. The most promising alternative power devices consist of vertical GaN devices, which often require regrown active regions. Here, we report on x-ray diffraction studies of the crystallinity of the GaN p-i-n structures prepared with and without ex-situ ambient exposure and/or chemical etching.
GaN for High Power Electronics

- Blue: LEDs and electric vehicles utilize silicon-based power electronics [1].
- Yellow: Power transmission and distribution require alternative approaches [1].

GaN outperforms Si, SiC with low on-resistance and high breakdown voltage [2].
Threading Dislocations (TDs)

Screw-type TDs

Edge-type TDs

Mosaic Tilt
Distortion of planes parallel to surface

Mosaic Twist
Distortion of angled planes

How can we quantify screw- and edge-type dislocation densities?

High Resolution X-ray Diffraction (HRXRD)

Bragg’s Law: \( n\lambda = 2dsin\theta_B \)

Diffraction plane normal

X-rays

Bragg angle \( \theta_B \)

\( 2\theta_B \)

\( \downarrow d \)

Symmetric \( \Delta \omega \) RC

Asymmetric \( \Delta \phi \) RC

X-rays

\( \Delta \omega \)

(0001)

Detector

\( \theta_B = \omega \)

\( \Delta \phi \)

(0001)

Detector
**Pseudo-Voigt Analysis of HRXRD**

\[
P(x) = I_0 [\eta C(x) + (1 - \eta) G(x)]
\]

\[
L_\parallel = \frac{0.9 \lambda}{\beta_\omega (0.017475 + 1.50048 \eta - 0.534156 \eta^2) \sin(\theta_B)}
\]

\[
\alpha_\omega = \beta_\omega [0.184446 + 0.812692 (1 - 0.998497 \eta)^{1/2} - 0.659603 \eta + 0.44554 \eta^2]
\]

**Screw TD density**

\[
N_S = \frac{\alpha_\omega^2}{2\pi b_S^2 \ln 2}
\]

**Edge TD Density**

\[
N_E = \frac{\alpha_\phi}{\sqrt{2\pi \ln 2} |b_E| L_\parallel}
\]

- \(P(x)\): Pseudo-Voigt function
- \(C(x)\): Cauchy profile
- \(G(x)\): Gaussian profile
- \(\eta\): Fitting parameter
- \(L_\parallel\): Lateral correlation length
- \(\beta_\omega\): \(\Delta \omega\) rocking curve FWHM
- \(\lambda\): X-ray wavelength
- \(\alpha_\omega\): Mosaic tilt angle
- \(b_S\): Screw TD Burger’s vector
- \(\alpha_\phi\): Mosaic twist angle
- \(b_E\): Edge TD Burger’s vector
Regrowth Interface at p-n Junction

**GaN Substrate**
- 2µm UID GaN
- 300µm n-GaN

**In-situ Regrowth**
- 300 nm p-GaN
- 2µm UID GaN
- 300µm n-GaN

**Ex-situ Regrowth**
- 300 nm p-GaN
  - Ex-situ air exposure
  - 2µm UID GaN
- 300µm n-GaN

**ICP Regrowth**
- 300 nm p-GaN
  - ICP etched
  - 2µm UID GaN
- 300µm n-GaN
Symmetric and Asymmetric Scans

(0004) X-rays \( \Delta \omega \) symmetric

(10\bar{1}5) X-rays \( \Delta \Phi \) asymmetric

Log X-ray Intensity

\( \Delta \omega \) (arcsec)

\( \beta_\omega \rightarrow \leftarrow \)

\( \Delta \Phi \) (deg)

\( \beta_\Phi \rightarrow \leftarrow \)
Structure & Electronic Properties Correlation

<table>
<thead>
<tr>
<th>Sample</th>
<th>$\delta \omega$ (arcsec)</th>
<th>$\eta$ (from $\Delta \omega$)</th>
<th>$\alpha_\omega$ ($10^{-4}$ rad)</th>
<th>$N_S$ ($10^6$ cm$^{-2}$)</th>
<th>$L_\parallel$ (µm)</th>
<th>$\delta \phi = \alpha_\phi$ ($10^{-4}$ rad)</th>
<th>$N_E$ ($10^8$ cm$^{-2}$)</th>
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<tr>
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<td>3.1</td>
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<td>108</td>
<td>6.3</td>
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</table>

Probing the structure using XRD:
- Ex-situ and ICP Etched had the largest screw-type TD densities
- In-situ had the lowest screw-type TD density and the highest edge-type TD density

Probing electronic properties using cathodoluminescence
- Donor acceptor pair emission (DAP) near the surface is lowest for Ex-situ and ICP Etched
- DAP emission at the regrowth interface is enhanced for ICP etched

Ambient air exposure worsens crystallinity and electronic properties, but ICP etching can partially restore the electronic properties.
Regrowth Interface in UID Layer

**GaN Substrate**
- 2μm UID GaN
- 300μm n-GaN

**Regrown Active Region**
- 15nm p+ GaN
- 200nm p-GaN
- 300nm UID GaN

**ICP**
- ICP etched
- 2μm UID GaN
- 300μm n-GaN

**ICP + TBCI**
- ICP etched + TBCI etched
- 2μm UID GaN
- 300μm n-GaN

**TBCI**
- TBCI etched
- 2μm UID GaN
- 300μm n-GaN
Symmetric Scans Only

Substrates
- UID GaN
- n-GaN

Log X-ray Intensity

ICP + TBCI
TBCI
ICP
Substrate

Regrowth
- UID GaN
- n-GaN

X-rays
$\Delta \omega$

Symmetric

$\beta_\omega$
## Probing the structure with XRD & RBS

<table>
<thead>
<tr>
<th>Sample</th>
<th>$\beta_\omega$ (arcsec)</th>
<th>$\eta$ (from $\Delta\omega$)</th>
<th>$\alpha_\omega$ (10^{-4} rad)</th>
<th>$N_S$ (10^6 cm^{-2})</th>
<th>$L_\parallel$ (µm)</th>
<th>$\beta_\phi = \alpha_\phi$ (10^{-4} rad)</th>
<th>$N_E$ (10^8 cm^{-2})</th>
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<tbody>
<tr>
<td>ICP + TBCl</td>
<td>70</td>
<td>0.059</td>
<td>3.2</td>
<td>8.5</td>
<td>6.6</td>
<td>0.0623 Å</td>
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<td>ICP + TBCl Regrowth</td>
<td>47</td>
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<td>2.5</td>
<td>0.0633 Å</td>
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</tr>
<tr>
<td>TBCl</td>
<td>37</td>
<td>0.372</td>
<td>1.2</td>
<td>1.1</td>
<td>2.6</td>
<td>0.0631 Å</td>
<td></td>
</tr>
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<td>TBCl Regrowth</td>
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<td>0.547</td>
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<td>0.7</td>
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<td>0.0623 Å</td>
<td></td>
</tr>
<tr>
<td>ICP</td>
<td>53</td>
<td>0.322</td>
<td>1.8</td>
<td>2.7</td>
<td>2.0</td>
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<td>ICP Regrowth</td>
<td>89</td>
<td>0.117</td>
<td>3.8</td>
<td>12.2</td>
<td>2.9</td>
<td>0.0631 Å</td>
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<tr>
<td>Substrate</td>
<td>48</td>
<td>0.201</td>
<td>1.9</td>
<td>3.0</td>
<td>3.3</td>
<td>0.0631 Å</td>
<td></td>
</tr>
</tbody>
</table>

**Future XRD work:**
- Conduct (10-15) phi scans
- Calculate twist angle
- Calculate edge-type TD density

### Probing the structure using XRD:
- **ICP** and **ICP Regrowth** had the largest screw-type TD densities

### Rutherford backscattering (RBS)
- RBS channeling maps allow us to determine the fraction of displaced Ga and N atoms
- **ICP** and **ICP Regrowth** had the largest fraction of displaced Ga and N atoms

XRD and RBS reveal **ICP Etching** lowers crystal quality overall.
References

5. “Linear Defects - Dislocations.” NDT Resource Center, National Science Foundation
Abstract

Although Si-based electronics are used to power light-emitting diodes and electric vehicles, their utility in high power applications is limited by a low breakdown voltage. The most promising alternative power devices consist of vertical GaN devices, which often require regrown active regions. Here, we report on x-ray diffraction studies of the crystallinity of the GaN p-i-n structures prepared with and without ex-situ ambient exposure and/or chemical etching. The full width at half max (FWHM) of phi and omega scans were used to quantify the mosaicity and threading dislocation (TD) densities at the p-i interfaces. The lowest screw-type and highest edge-type TD densities are observed for the “in-situ” GaN structure, which also produces the highest interfacial near-band edge (NBE) and donor-acceptor pair (DAP) cathodoluminescence (CL) emissions. Interestingly, elastic recoil detection analysis (ERDA) and Rutherford backscattering spectroscopy reveal the lowest interfacial [H] but the highest fraction of displaced Ga atoms, suggesting efficient incorporation of Mg$_{Ga}$ in the in-situ structure. On the other hand, for the ex-situ structures, minimal interfacial [H] is also observed, but the lowest interfacial NBE and DAP CL emission is apparent as well as the highest screw-type TD density. The relationship between interfacial [H], displaced Ga, CL emission features, and screw- and edge-type dislocation densities will be discussed.
The Pseudo-Voigt function, $P(x)$, approximates the convolution of Cauchy, $C(x)$, and Gaussian, $G(x)$, profiles and is given by equations (1):

$$P(x) = I_0[\eta C(x) + (1 - \eta)G(x)]$$

and $0 \leq \eta \leq 1$, where $\eta$ is a fitting parameter [6]. The lateral correlation length, $L_\parallel$, and tilt angle, $\alpha_\omega$, can then be calculated using equations (2) and (3), respectively:

$$L_\parallel = \frac{0.9\lambda}{\beta_\omega(0.017475 + 1.50048\eta - 0.534156\eta^2)\sin(\theta_B)}$$

$$\alpha_\omega = \delta_\omega[0.184446 + 0.812692(1 - 0.998497\eta)^{1/2} - 0.659603\eta + 0.44554\eta^2]$$

where $\lambda$ is the x-ray wavelength, $\delta_\omega$ is the FWHM of the $\Delta \omega$ rocking curve, and $\theta_B$ is the Bragg angle [6].

$$N_S = \frac{\alpha_\omega^2}{2\pi b_S^2 \ln 2}$$

$$N_E = \frac{\alpha_\phi}{\sqrt{2\pi \ln 2} |b_E| L_\parallel}$$