Channelling Theory and Simulation

• Channelling Applications

• The FLUX Code

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Outline

• **Introduction:**
  - Rutherford Backscattering and Channelling (RBS/C)
  - III-Nitrides

• **Characterisation of III-N structures from 3D to 0D:**
  - 3D Thin films (crystal quality, strain, ion implantation damage, lattice site location of dopants)
  - 2D Quantum wells (crystal quality, strain)
  - 1D Nanowires (mosaicity)
  - 0D Quantum dots (crystal quality, strain)

• **The FLUX Code**

• **Summary**
Concept

- Mass perception (kinematic factor)
- Concentration (x-section)
- Depth resolution (stopping force)
Ion-Channelling

“Channelling of energetic ions occurs when the beam is carefully aligned with a major symmetry direction of a single crystal.” [Lindhard 1965]

- Reduction of yield up to 98%
- Lattice position of impurities (interstitial or substitutional)
- Sensitive to disorder, lattice mismatch, strain, defects etc.
Ion-Channelling

Schematic of particle trajectories undergoing scattering at the surface and channeling within the crystal. The depth scale is compressed relative to the width of the channel in order to display the trajectories.
Ion-Channelling – Critical Angle

- Channelled ion
- Ion backscattered at surface
- Backscattering or dechannelling takes place when the incident angle is higher than the critical angle for channelling.
• Minimum yield: related with the crystal quality (blocked area).
• Half-width angle: related with the critical angle for channeling.
Rutherford Backscattering /Channelling

- Elemental depth profile
- Compositional quantification
- Interface and growth problems
- No standards, non-destructive

- Damage profile
- Lattice defects
- Amorphous layers
- Strain in epitaxial films
### RBS/C Lattice Site Location

![Diagram of lattice site location with arrows indicating directions and shaded squares indicating shadowed fractions.]

<table>
<thead>
<tr>
<th>Shadowed Fraction</th>
<th>(&lt;10\rangle)</th>
<th>(&lt;11\rangle)</th>
<th>(&lt;1-1\rangle)</th>
</tr>
</thead>
<tbody>
<tr>
<td>substitutional</td>
<td>100 %</td>
<td>100 %</td>
<td></td>
</tr>
<tr>
<td>interstitial</td>
<td>50 %</td>
<td>0 %</td>
<td></td>
</tr>
<tr>
<td>interstitial</td>
<td>0 %</td>
<td>100 %</td>
<td></td>
</tr>
</tbody>
</table>

**Note:** The diagram illustrates the location of shadowed fractions for substitutional and interstitial sites in a lattice structure, with specific percentages indicating the fraction of sites shaded for each orientation.
Group-III Nitrides

AlGaN: UV emitters/
Detectors
HEMTS

InGaN:
LEDs, LASERS

AlInN: - Widest energy range
- Lattice-match to GaN

InGaN:
LEDs, LASERS

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UV emitters/
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InGaN: - Widest energy range
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AlGaN
InGaN
Bandgap (eV)
a Lattice Constant (Å)
AlN
GaN
InN
Al\textsubscript{1-x}In\textsubscript{x}N x\approx 17-18 \%

Al\textsubscript{1-x}In\textsubscript{x}N
Samples

Al$_{1-x}$In$_x$N

- Growth by MOCVD
- Substrate: GaN on (0001) sapphire
- Thickness: ~100 nm

Biaxial strain

Al$_{1-x}$In$_x$N

GaN (1-6 µm)
sapphire
Crystal Quality of thin films

Composition, thickness and crystal quality

⇒ Good crystal quality for InN contents < ~20% (Minimum yields 3-6%)
Example AlInN/GaN bi-layers

Growth at 840 °C

Growth at 760 °C

Good crystalline quality

Worse crystalline quality
Measuring Strain by RBS/C

\[ \varepsilon_{\tau} = \frac{\Delta \Phi}{\sin \Phi \cos \Phi} \]

\[ \varepsilon_{\tau} = \varepsilon_{\parallel} - \varepsilon_{\perp} \]

Tetragonal distortion:

\[ \varepsilon_{\parallel} = \frac{a_{\text{epi}} - a_{\text{rel}}}{a_{\text{rel}}} \]

\[ \varepsilon_{\perp} = \frac{c_{\text{epi}} - c_{\text{rel}}}{c_{\text{rel}}} \]

\[ \tan \Phi = \frac{a}{c} \]

Lorenz et al. PRL 97 (2006) 85501
Lorenz et al. JCG 310 (2008) 4058

SPRITE Workshop
Depth dependent strain measurement
Energy windows (W) select different depths

Surface layer is relaxed
Deeper region under compressive strain

⇒ Relaxation via change of composition
Strain Relaxation: Compressive Strain

Depth dependent strain measurement
Energy windows (W) select different depths

Relaxation towards the surface

⇒ Relaxation via change of c/a ratio (constant composition)
Morphology Change

Pseudomorphic
\[ x = 0.16 \]

Partly relaxed
\[ x = 0.22 \]

Relaxed
\[ x = 0.24 \rightarrow 0.19 \]

RMS = 0.6 nm

RMS = 2.1 nm

RMS = 6.2 nm

Roughening/3D growth
“Anomalous” features like double-dips

InN content 15%

R: angle for relaxed AlInN → determined from Vegard´s law
Steering effects in the interface

Angular scan of GaN substrate distorted when kink angle ≤ critical angle
→ $\alpha$-energy
→ kink angle (InN content)
Steering effects: FLUX Simulations

Different kink angles

Different energies

Increasing beam energy
Comparison with simulations

Redondo-Cubero, Lorenz et al. APL 95 (2009) 051921
Redondo-Cubero, Lorenz et al. JPD 42 (2009) 065420
GaN Scans and FLUX Simulations

ΔΦ = 0.3°
ΔΦ = 0.5°
ΔΦ = 0.66°

19% InN
15% InN
13% InN

<2113>
<10-11>
Strain Analysis XRD - RBS

XRD
\[ \varepsilon_\tau = \varepsilon^\parallel - \varepsilon^\perp \]

RBS
\[ \varepsilon_\tau = \frac{\Delta \Phi}{\sin \phi \cos \phi} \]

Perfect Lattice matching for \( x=0.171 \)

Lorenz et al. PRL 97 (2006) 85501
Implantation damage in GaN

$3 \times 10^{15}$ at/cm$^2$ Eu implantation 300 keV at RT

$\Rightarrow$ 2 damage regions (surface / bulk)
Implantation damage in GaN

$$\Delta \chi_{\text{min}} = \frac{\gamma_{\text{aligned implanted}} - \gamma_{\text{aligned as-grown}}}{\gamma_{\text{random}}}$$

⇒ RBS/C aligned spectra need correction for dechannelling
(in this case using the DICADA program, Gärtner et al. NIMB 216 (1983) 275; 227 (2005) 522)
GaN:Eu grown by MOCVD at 1000°C

→ Homogeneous Eu distribution with depth ~0.1 at% 
→ Excellent crystal quality (Minimum yield <3%)
Lattice site location of Eu in GaN

→ Eu incorporated to ~100% on Ga-sites
→ Eu displaced (0.2 Å) for sample grown at 900°C
→ Eu clusters

Lorenz et al. APL 97 (2010) 111911
Group-III Nitride Nanostructures

**2D**
InGaN/GaN quantum wells (QW)

**1D**
GaN nanowires (NW)

**0D**
GaN quantum dots (QD)

- **LED**
  - p-electrode
  - semi-transparent contact layer
  - p-GaN:Mg
  - p-AlGaN:Mg EBL
  - active region
  - n-GaN:Si
  - n-electrode

- **InGaN QW**
  - 2-3 nm

- **GaN nanowires**
  - 100 nm

- **GaN quantum dots**
  - 15 nm
  - 5 nm
Problems when going to nano-scale

Limited depth resolution in conventional RBS (~20nm)

Problems:
- Besides thickness and composition, is the width of the peak dependent on:
  - Energy resolution
  - Intermixing of layers
  - Roughness

→ In case of ambiguities need of complementary experimental techniques (TEM, AFM...)

⇒ Grazing incidence
GaN QD / AlN Multilayers

150 bilayers

- GaN QD: 6ML
- AlN spacer: ~8 nm
- AlN (10nm)
- SiC

Grown by MBE using the Stranski-Krastanow growth mode

RBS Normal Incidence

Random and <0001> aligned

Scan across <0001>

⇒ Excellent crystalline quality along c-axis $\chi_{\text{min}}=4\%$!
Crystal Quality of QDs

Crystal quality of each QD plane can be assessed and does not change with depth.

QD at surface show reduced channelling probably due to strain relaxation and oxidation.
**Buried SQW / SQD-plane**

<table>
<thead>
<tr>
<th>Layer Structure</th>
<th>RBS</th>
<th>XRR</th>
</tr>
</thead>
<tbody>
<tr>
<td>AlN cap QD</td>
<td>8.9 (1.0) nm</td>
<td>9.4 nm</td>
</tr>
<tr>
<td>QD</td>
<td>2.6 nm (V_f=27%)</td>
<td>0.46 nm</td>
</tr>
<tr>
<td>AlN cap SQW</td>
<td>8.1(1.0) nm</td>
<td>8.8 nm</td>
</tr>
<tr>
<td>SQW</td>
<td>0.6 (1) nm</td>
<td>0.54 nm</td>
</tr>
</tbody>
</table>
Crystal quality better in QD than in QW

Formation of misfit defects?
- misfit (GaN-AlN 2.5%) can lead to formation of dislocations and stacking faults as evidenced by TEM analysis (Kandaswamy et al. JAP 106 (2009) 013526)
Strain measurement: thin film

\[ \varepsilon = \frac{\Delta \Phi}{\sin \Phi \cos \Phi} \]

Al\(_{1-x}\)In\(_x\)N

GaN (1000 nm)

sapphire

Problems when going to nano-scale

For example a buried GaN single quantum well (SQW) in AlN

\[ \text{AlN} \]
\[ 10 \text{ nm} \]
\[ \text{GaN SQW} \]
\[ 3.5 \text{ ML} \]
\[ \text{AlN} \]
\[ 26 \text{ nm} \]
\[ \text{SiC} \]

⇒ The GaN SQW is too thin to exhibit channelling effects on the beam
⇒ Ga-atoms act like an impurity
  Scans do not shift but show asymmetries and flux peaking
0.9 nm QW \( \Rightarrow \Delta \theta = 0.14^\circ \Rightarrow \varepsilon_T = -3.9\% \)
0.6 nm QW \( \Rightarrow \Delta \theta = 0.22^\circ \Rightarrow \varepsilon_T = -7\% \)

\( \varepsilon_T \text{ (fully strained)} = -3.6\% \)

\( \Rightarrow \) QD partly relaxed but error in current data analysis is extremely high

\( \Rightarrow \) MC simulations need to include sample imperfections and QD

0.9 nm QD \( \Rightarrow \Delta \theta = 0.12^\circ \Rightarrow \varepsilon_T = -3.1\% \)
1.7 nm QD \( \Rightarrow \Delta \theta = 0.7^\circ \Rightarrow \varepsilon_T = -1.6\% \)
2.6 nm QD \( \Rightarrow \Delta \theta = 0.5^\circ \Rightarrow \varepsilon_T = -0.4\% \)

\( \varepsilon_T \text{ (Raman, XRD)} = -2.4\% \)
(Cros et al. PRB 76 (2007) 165403)
## High resolution RBS or MEIS

<table>
<thead>
<tr>
<th></th>
<th>RBS</th>
<th>HR-RBS / MEIS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Energy</td>
<td>~ 1-5 MeV (α, p)</td>
<td>~ 50-500 keV (α, p)</td>
</tr>
<tr>
<td>Detector system</td>
<td>Si surface barrier detector</td>
<td>Electrostatic analyser or magnetic spectrometer:</td>
</tr>
<tr>
<td>Resolution</td>
<td>~ 15 keV</td>
<td>&lt; 1 keV</td>
</tr>
<tr>
<td>Detector system</td>
<td>~10 nm</td>
<td>&lt; 1 nm</td>
</tr>
<tr>
<td>Probing depth</td>
<td>~1 μm</td>
<td>~20 nm</td>
</tr>
</tbody>
</table>

### Conventional RBS
- Incident Beam
- Scattered Ion
- SSD

### HRBS
- Diversion Magnet
- SLIT
- High Energy Ion
- Low Energy Ion
- Scattered Ion
- Sample
- Position Detector (MCP+PSD)

### MEIS
- Position sensitive detector
- Electrostatic analyzer
MEIS: Strain distribution in GaN QDs

Blocking

$\Rightarrow$ QD relax towards the top of the pyramid

Jalabert et al. PRB 72 (2005) 115301
RBS/C on nanowires?

- Vertically aligned NW grown by MBE on 111 Si
Alignment of Nanowires

- Preferential orientation of nanowires:
  
  \[
  [111] \text{Si} \parallel [0001] \text{GaN} \\
  [11-2] \text{Si} \parallel [10-10] \text{GaN}
  \]
Mosaicity of Nanowires

Ion channelling in NWs allows determination of orientation, tilt and twist via Monte Carlo simulations:

- Tilt: 0.4°
- Twist: 0.5°
Implantation damage in GaN

Eu implantation 300 keV at RT

⇒ Sigmoidal shaped damage build-up curve
⇒ Efficient dynamic annealing

Implantation damage in GaN

- Point defect clusters
- Low concentration of stacking faults
Implantation damage in GaN

HRTEM

- Increasing number of stacking faults
Implantation damage in GaN

- Nanocrystalline surface layer with voids
- Stacking fault density in bulk saturates
\( \text{In}_x\text{Ga}_{1-x}\text{N}/\text{GaN}: \) Thin film

Fit results:
50 nm \( \text{In}_{15.9}\text{Ga}_{84.1}\text{N} \)

\( \Rightarrow \) A fit (e.g. using the NDF code) gives the thickness and composition of the film and can give information on compositional gradients, roughness, contaminations etc.
**In$_x$Ga$_{1-x}$N/GaN: Manual Analysis**

**Fit results:**

50 nm In$_{0.159}$Ga$_{0.841}$N

Experimental data and fit overlap closely, indicating a good match.

- **Counts (Y$_i$):**
  - N: 2550 cnts
  - Ga: 1220 cnts

**Composition Calculation:**

\[
Y_i \propto \sigma_r \cdot N_i \quad \Rightarrow \quad [N_i] = \frac{at}{cm^2}
\]

\[
\frac{N_{\text{In}}}{N_{\text{Ga}}} = \frac{Y_{\text{In}} \cdot \sigma_r (\text{Ga})}{Y_{\text{Ga}} \cdot \sigma_r (\text{In})}
\]

\[
= \frac{1220 \cdot 2.482264 \text{ barn/str}}{2550 \cdot 6.221996 \text{ barn/str}} = 0.191
\]

**Equations:**

\[
N_{\text{In}} = \frac{x}{1 - x} \quad \Rightarrow \quad x = \frac{N_{\text{In}}}{N_{\text{Ga}}} = 0.16
\]

**Conclusion:**

Composition from fit and manual analysis match perfectly.
For very thin layers the height of the In-peak depends not only on composition but also on the thickness of the layer due to the limited depth resolution.
In$_x$Ga$_{1-x}$N/GaN: Multi Quantum Well (MQW)

5 samples with different InN content

In$_x$Ga$_{1-x}$N/GaN MQW
5 periods
Nominal QW thickness 3nm
Grown by Metal Organic Chemical Vapour Deposition (MOCVD)

$\Rightarrow$ QW thickness and QW composition difficult to measure with most techniques

- XRD measured the period and average composition
- PIXE, WDX measures the total In-content; QW thickness needs to be known
- SIMS suffers from artefacts due to contaminations from the sides
- TEM+EDX possible but very time consuming
**In$_{x}$Ga$_{1-x}$N/GaN: Multi Quantum Well (MQW)**

⇒ Composition and thickness cannot be determined unambiguously
  (complementary measurements necessary e.g. TEM).
⇒ Period, total InN content and “product” thickness × composition.
⇒ Assuming the nominal thickness of 3 nm, x was determined to vary from 2 to 14 %
Minimum yield for Ga: < 2% in all samples

Minimum yield for In: 2-10% (better for thinner GaN barrier layers)
**Grazing Incidence**

Tilt 86°

![Graph of Tilt 86° with Al and Ga peaks, showing Fit and Experimental Data.]

<table>
<thead>
<tr>
<th>Layer</th>
<th>Material</th>
<th>Thickness [nm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>GaN/AlN</td>
<td>3.435</td>
</tr>
<tr>
<td>2</td>
<td>AlN</td>
<td>4.558</td>
</tr>
<tr>
<td>3</td>
<td>GaN/AlN</td>
<td>2.669</td>
</tr>
<tr>
<td>4</td>
<td>AlN</td>
<td>5.202</td>
</tr>
<tr>
<td>5</td>
<td>GaN/AlN</td>
<td>2.642</td>
</tr>
<tr>
<td>6</td>
<td>AlN</td>
<td>5.082</td>
</tr>
<tr>
<td>7</td>
<td>GaN/AlN</td>
<td>2.557</td>
</tr>
<tr>
<td>8</td>
<td>AlN</td>
<td>5.037</td>
</tr>
<tr>
<td>9</td>
<td>GaN/AlN</td>
<td>2.663</td>
</tr>
</tbody>
</table>

Input:

Cylindrical QD: Height 2.6 nm
Radius 8.5 nm

⇒ QD volume fraction 40%
Simulating QD with NDF

- NDF\(^1\) (IBA Data Furnace) spherical\(^2\) and cylindrical\(^3\) QD
  → cylindrical QD: Height 2.6 nm
  Radius 8.5 nm

NDF calculates:
- Quantity of material crossed
- Energy spread due to difference in stopping power

→ volume fraction

\(^{1}\)N. Barradas et al. APL 71 (1997) 291.
\(^{3}\)N. Barradas et al. unpublished
Volume fraction of GaN QD

⇒ Volume-fraction of GaN QD: 0.4
⇒ Good agreement with TEM
⇒ Uncovered QDs at surface are bigger
  (confirmed by TEM, Gogneau et al. JAP 96 (2004) 1104)