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)

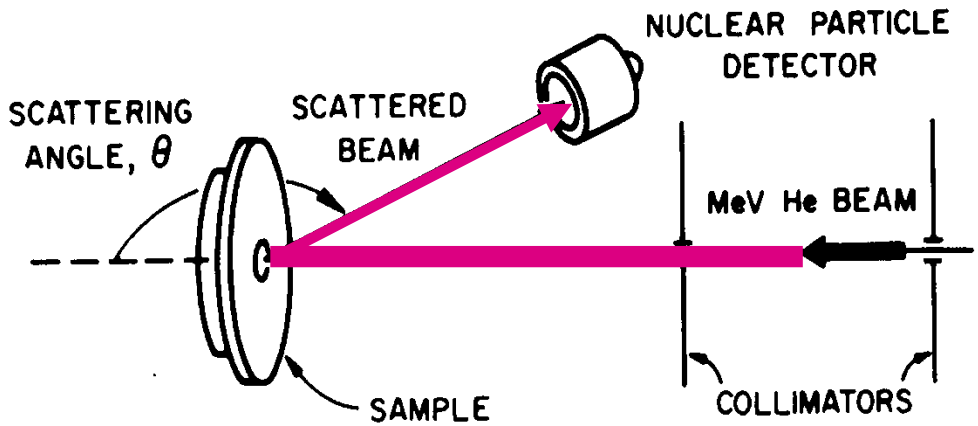
- **The FLUX Code**

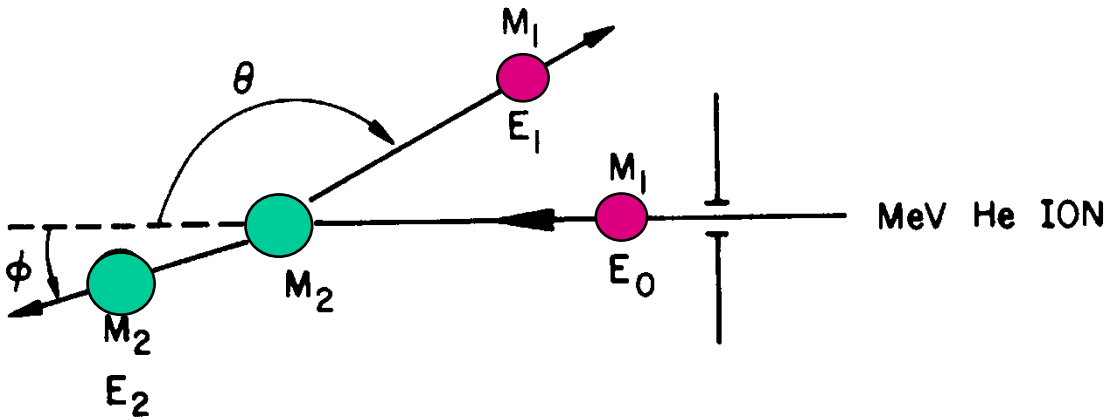
- **Summary**

RBS

Concept

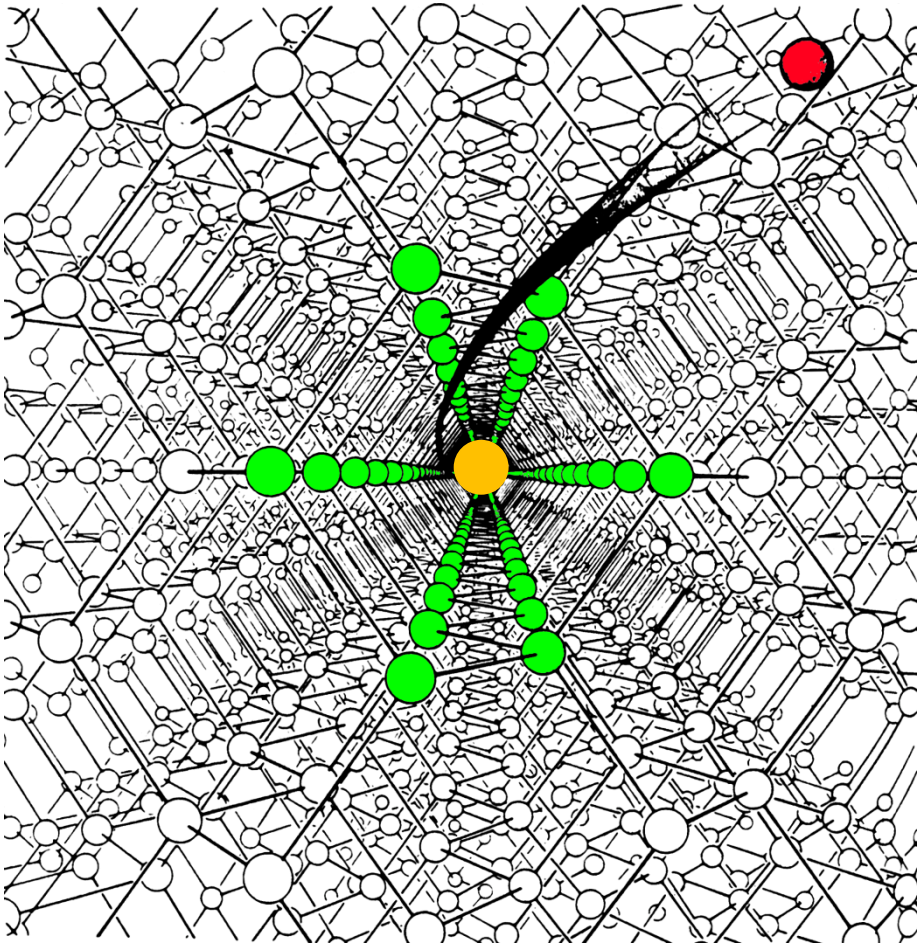
+ Mass perception (kinematic factor)
+ Concentration (x-section)
+ Depth resolution (stopping force)





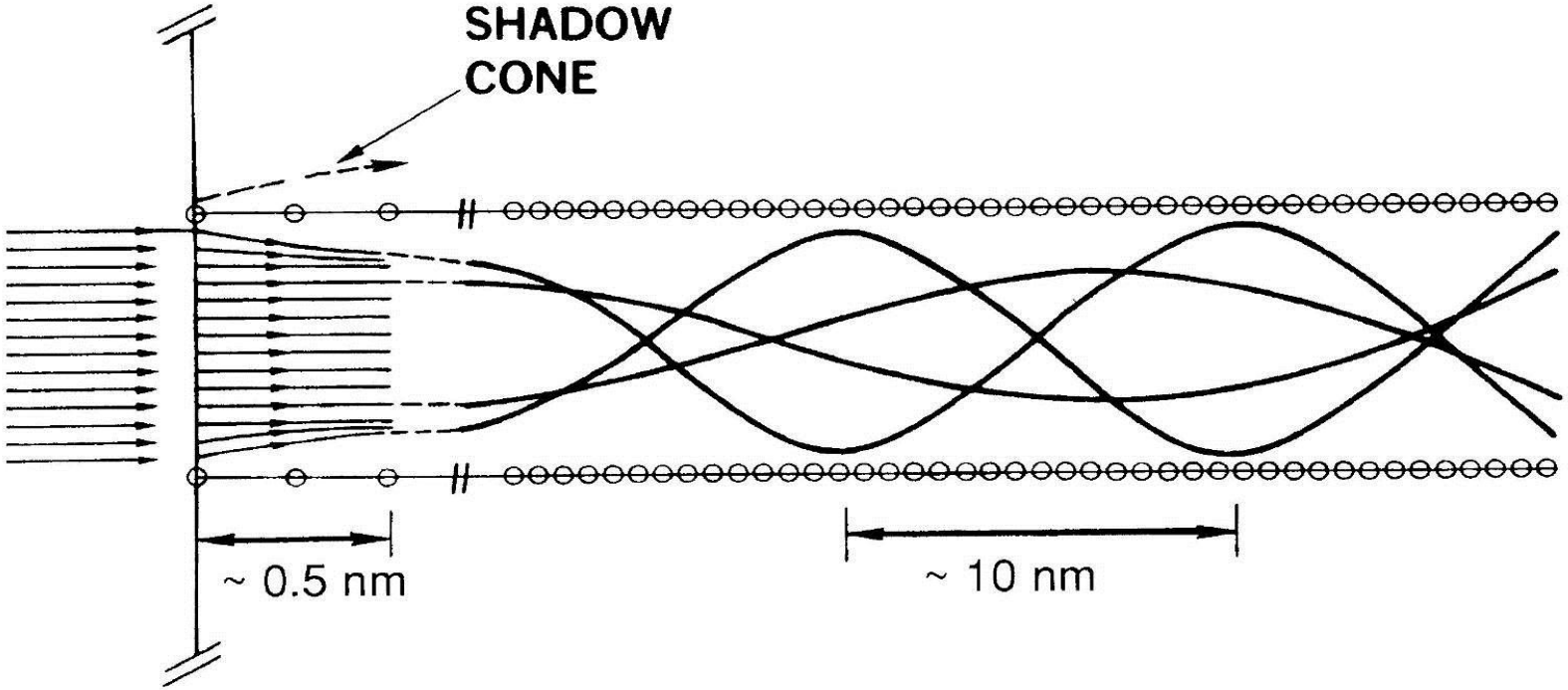
Ion-Channelling

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



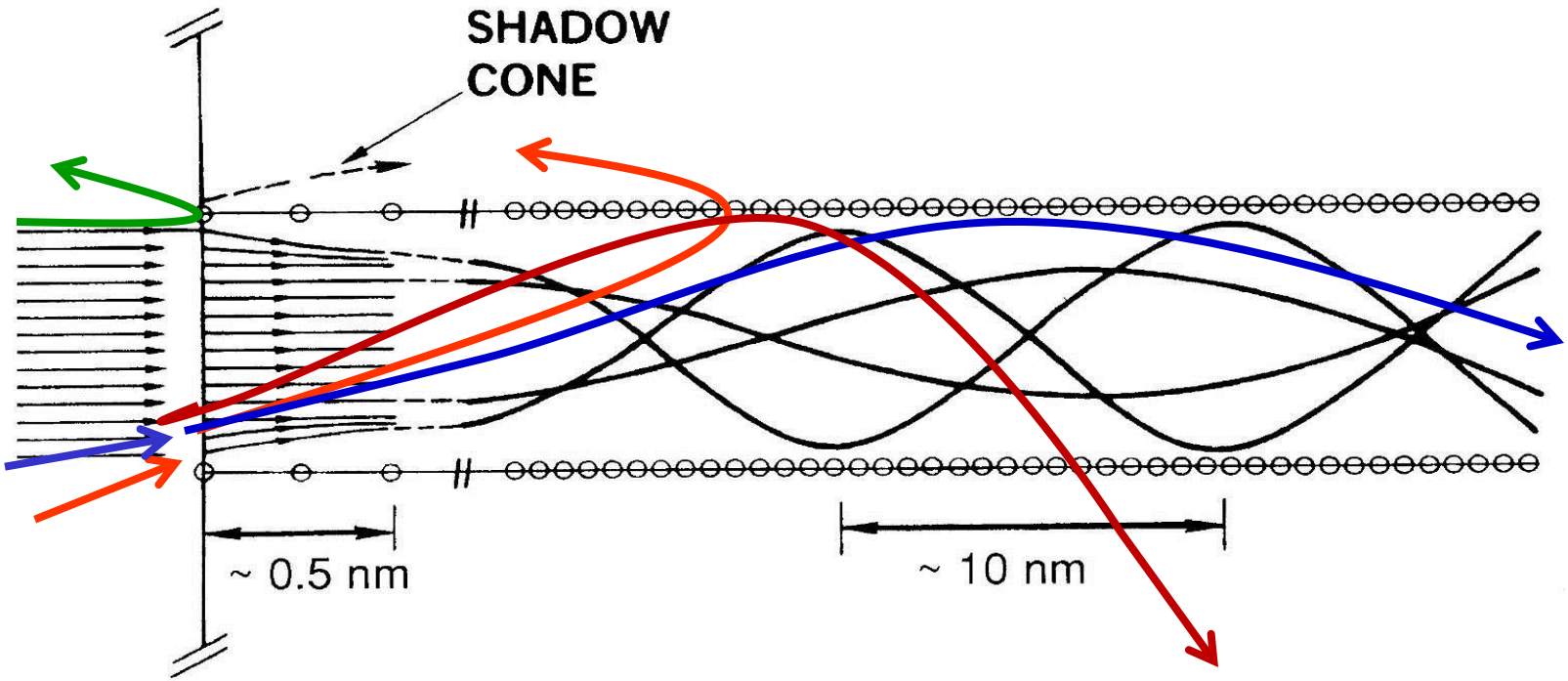
- Reduction of yield up to 98%
- Lattice position of impurities (interstitial or substitutional)
- Sensitive to disorder, lattice mismatch, strain, defects etc.

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

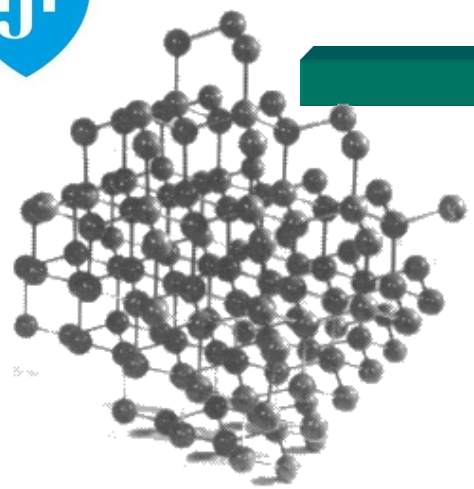


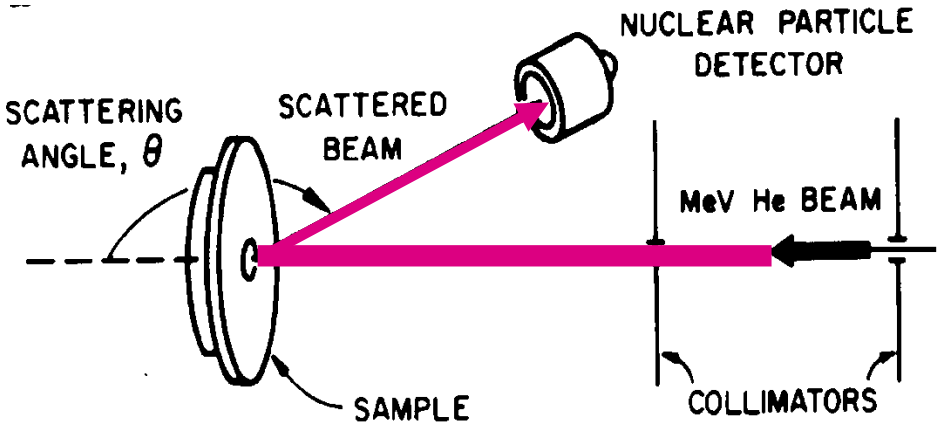
⇒ Channelled ion

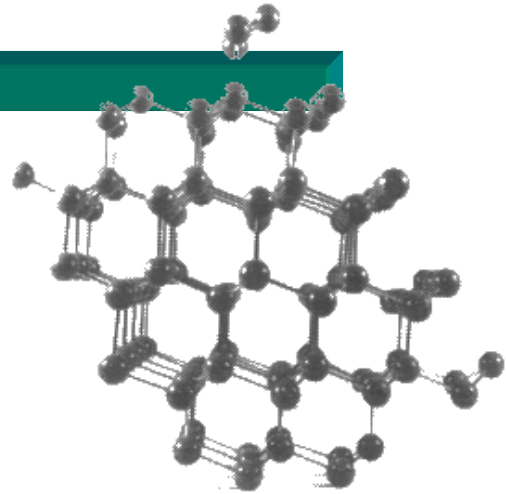
⇒ Ion backscattered at surface

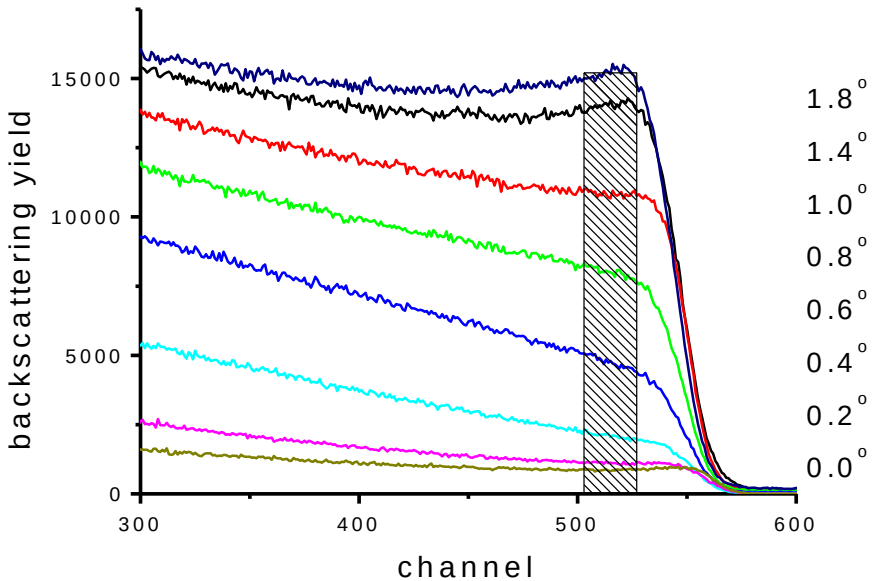
⇒ Backscattering or dechannelling takes place when the incident angle is higher than the critical angle for channelling.

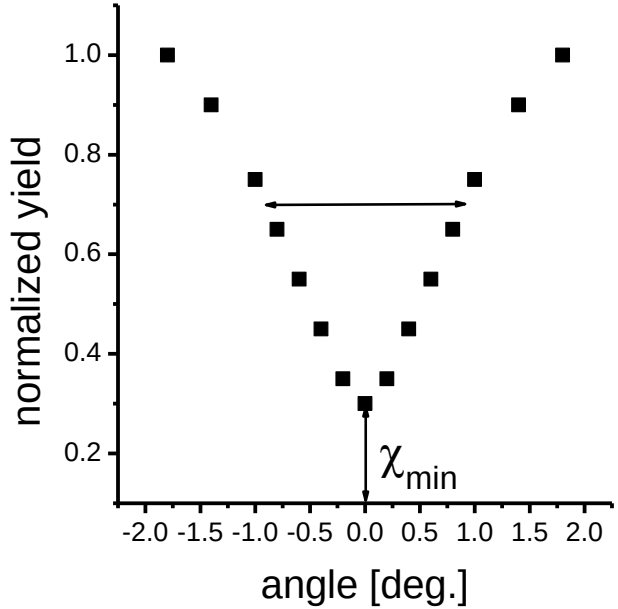
RBS-Channelling





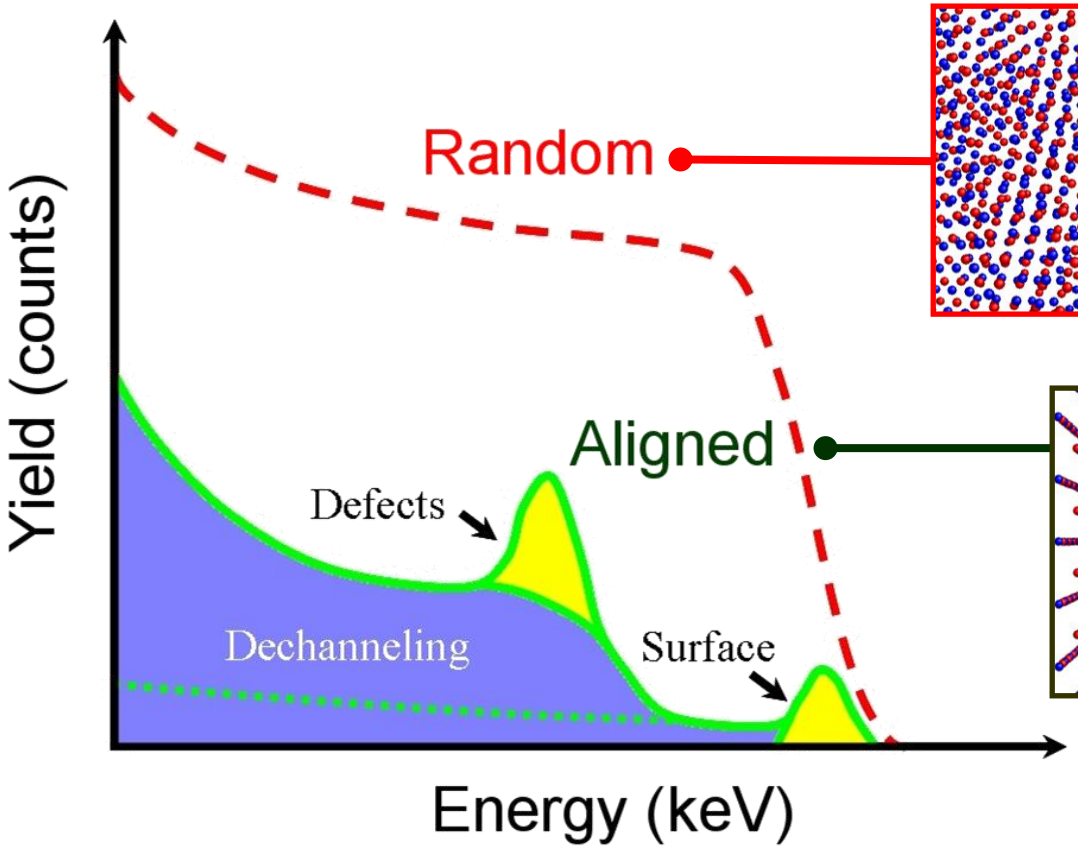


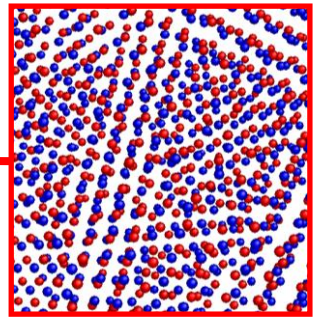




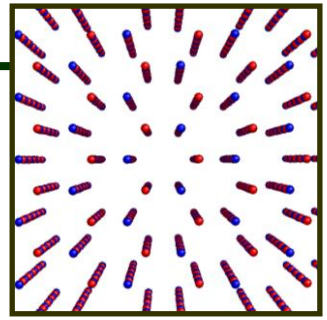
- Minimum yield: related with the crystal quality (blocked area).
- Half-width angle: related with the critical angle for channeling.

Rutherford Backscattering /Channelling



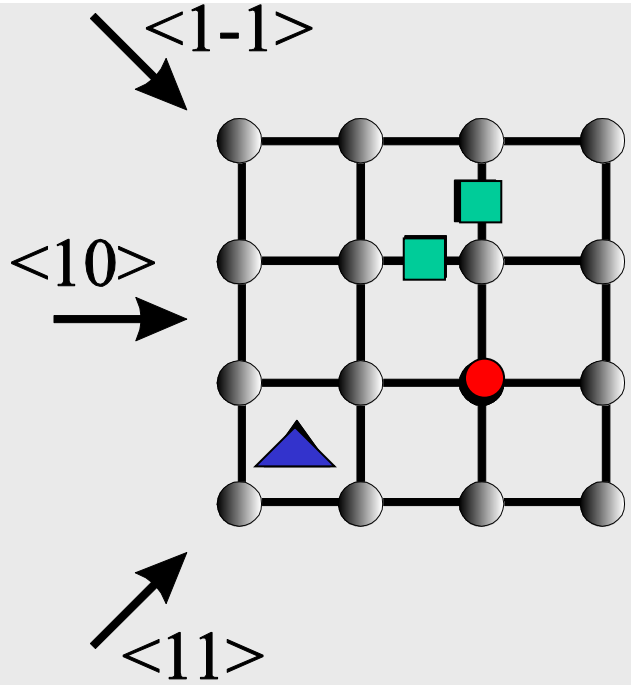


- **Elemental depth profile**
- Compositional quantification
- Interface and growth problems
- No standards, non-destructive



- **Damage profile**
- Lattice defects
- Amorphous layers
- Strain in epitaxial films

RBS/C Lattice Site Location



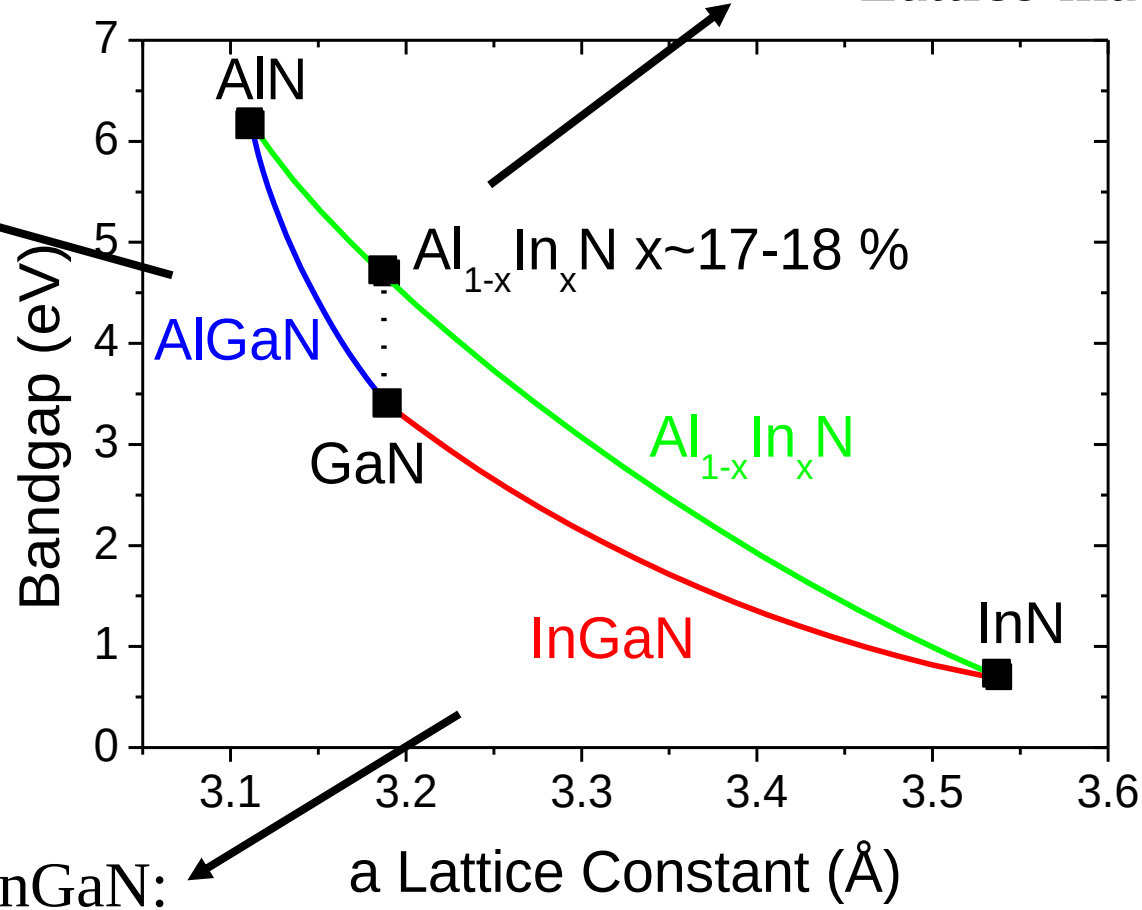
Shadowed fraction

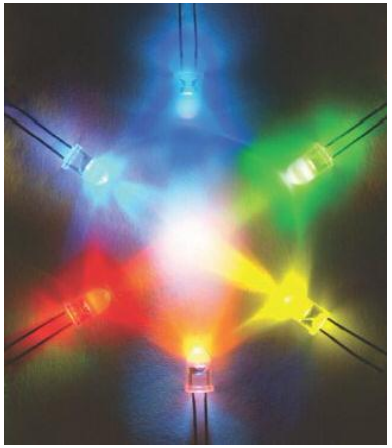
		<10>	<11> <1-1>
substitutional	●	100 %	100 %
interstitial	■	50 %	0 %
interstitial	▲	0 %	100 %

Group-III Nitrides

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

AlGaN:
UV emitters/
Detectors
HEMTS



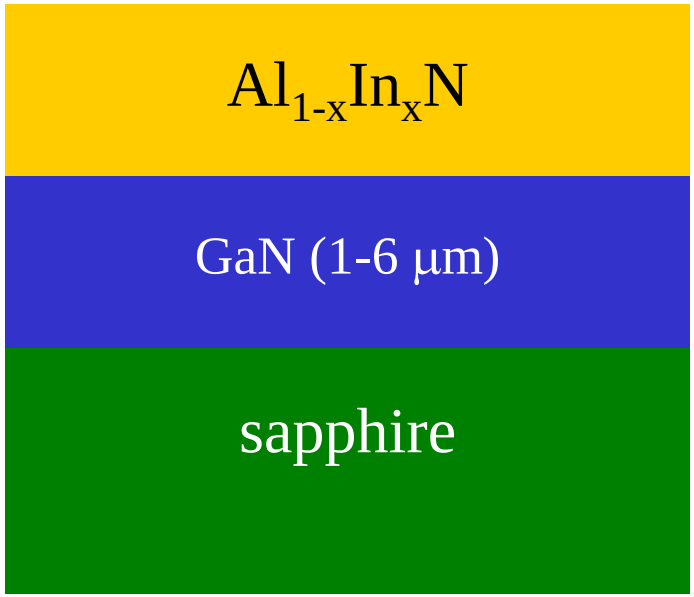


InGaN:
LEDs, LASERS

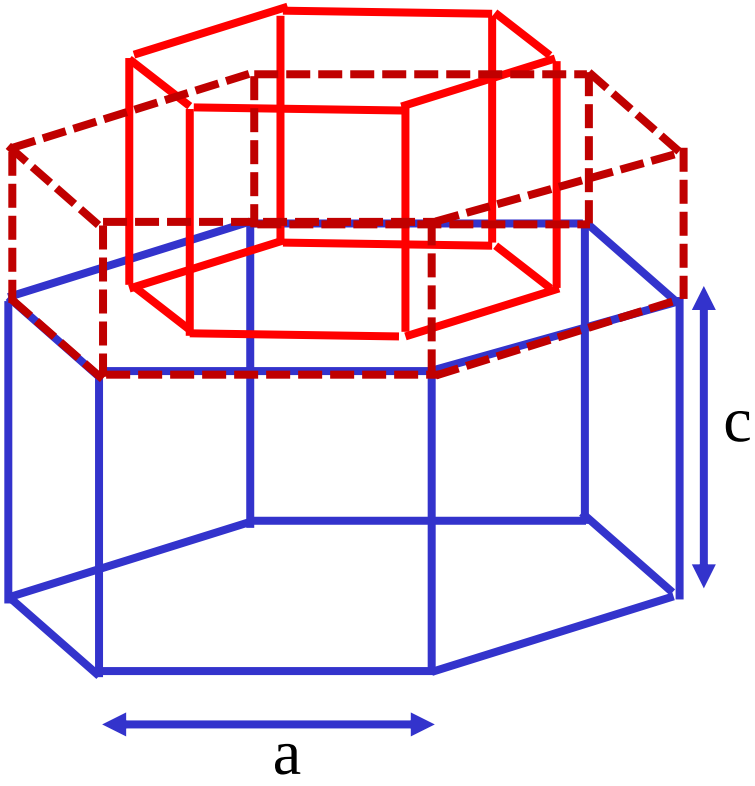
Samples

$Al_{1-x}In_xN$

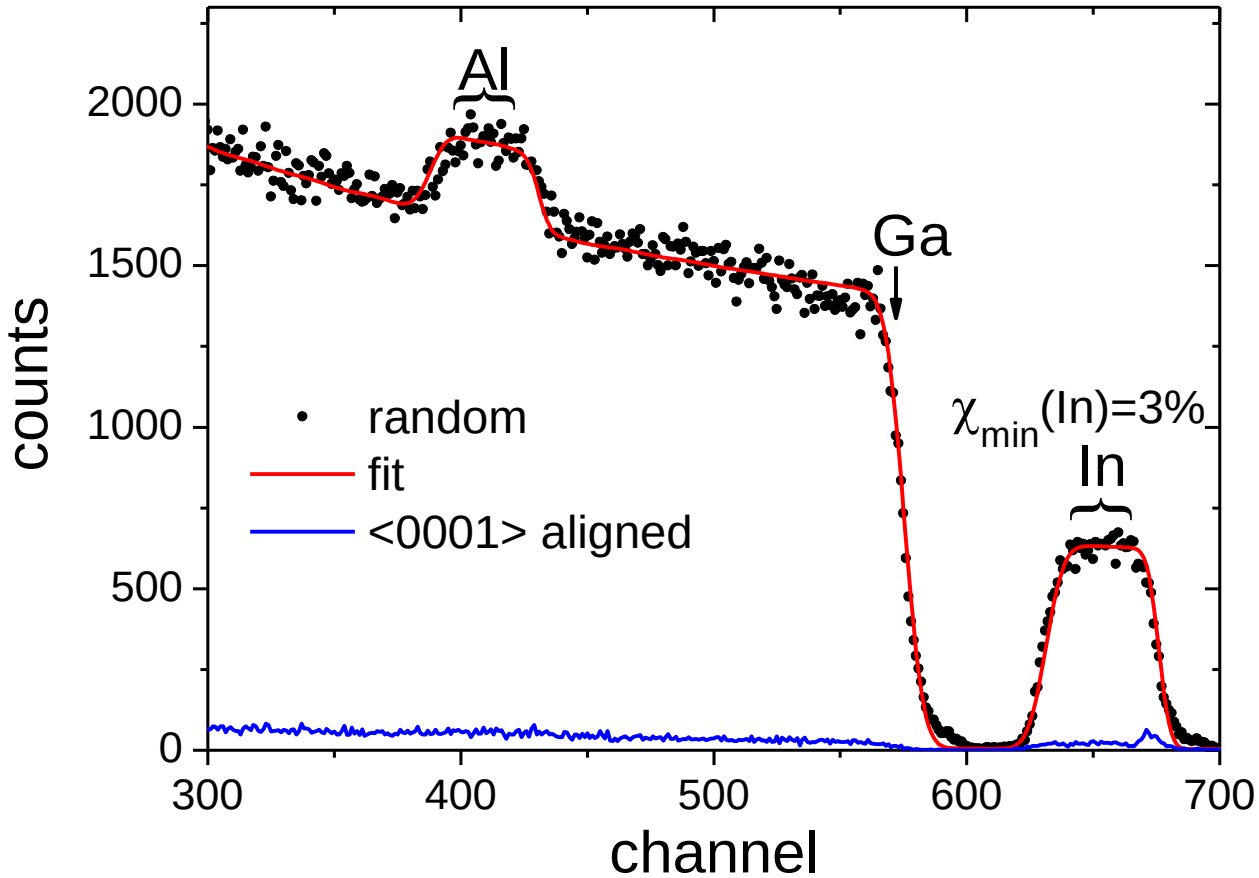
- Growth by MOCVD
- Substrate: GaN on (0001) sapphire
- Thickness: ~100 nm



Biaxial strain



Crystal Quality of thin films

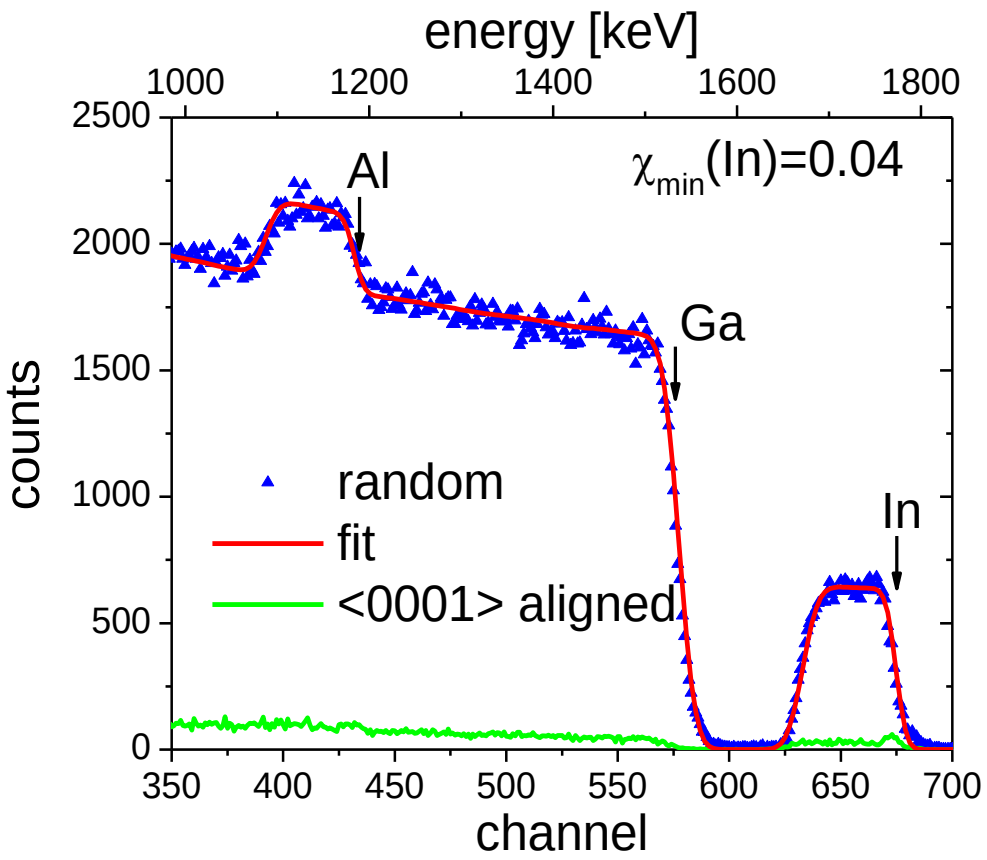


⇒ Composition, thickness and crystal quality

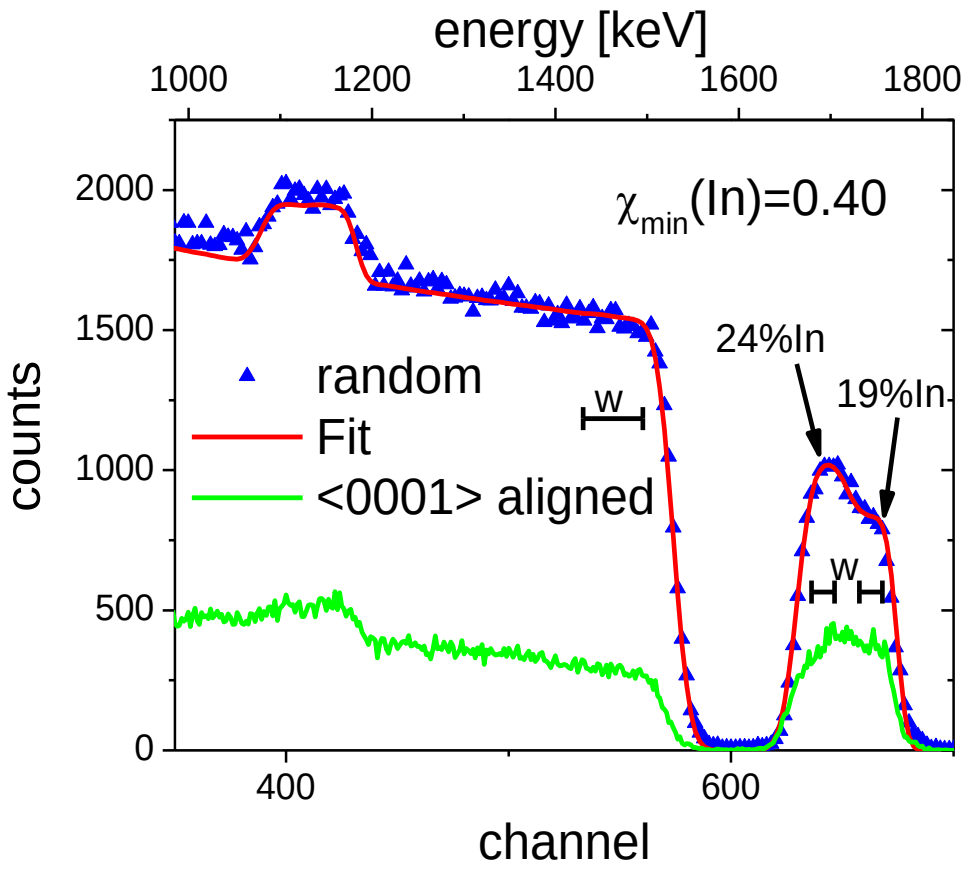
⇒ Good crystal quality for InN contents < ~20% (Minimum yields 3-6%)

Example AlInN/GaN bi-layers

Growth at 840 ºC



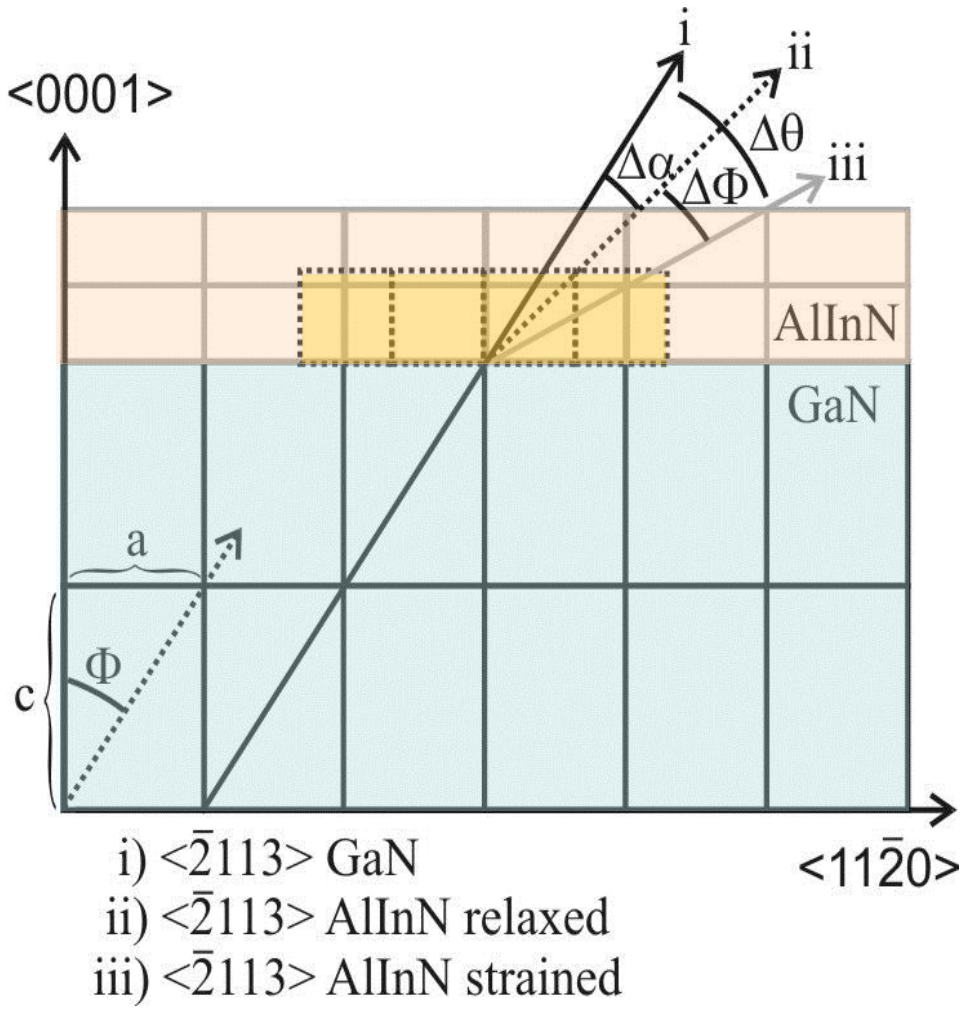
Growth at 760 ºC



Good crystalline quality

Worse crystalline quality

Measuring Strain by RBS/C



$$\tan \Phi = \frac{a}{c}$$

Tetragonal distortion:

$$\varepsilon_\tau = \frac{\Delta\Phi}{\sin \Phi \cos \Phi}$$

$$\varepsilon_\tau = \varepsilon^{\parallel} - \varepsilon^{\perp}$$

$$\varepsilon^{\parallel} = \frac{a_{epi} - a_{rel}}{a_{rel}}$$

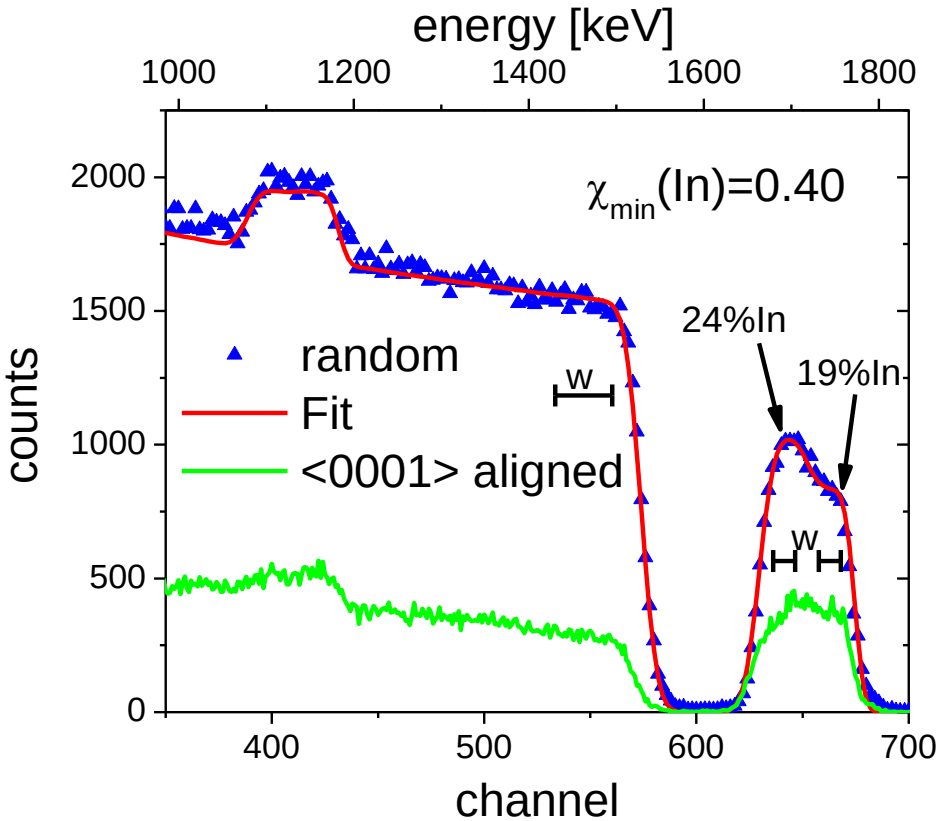
$$\varepsilon^{\perp} = \frac{c_{epi} - c_{rel}}{c_{rel}}$$

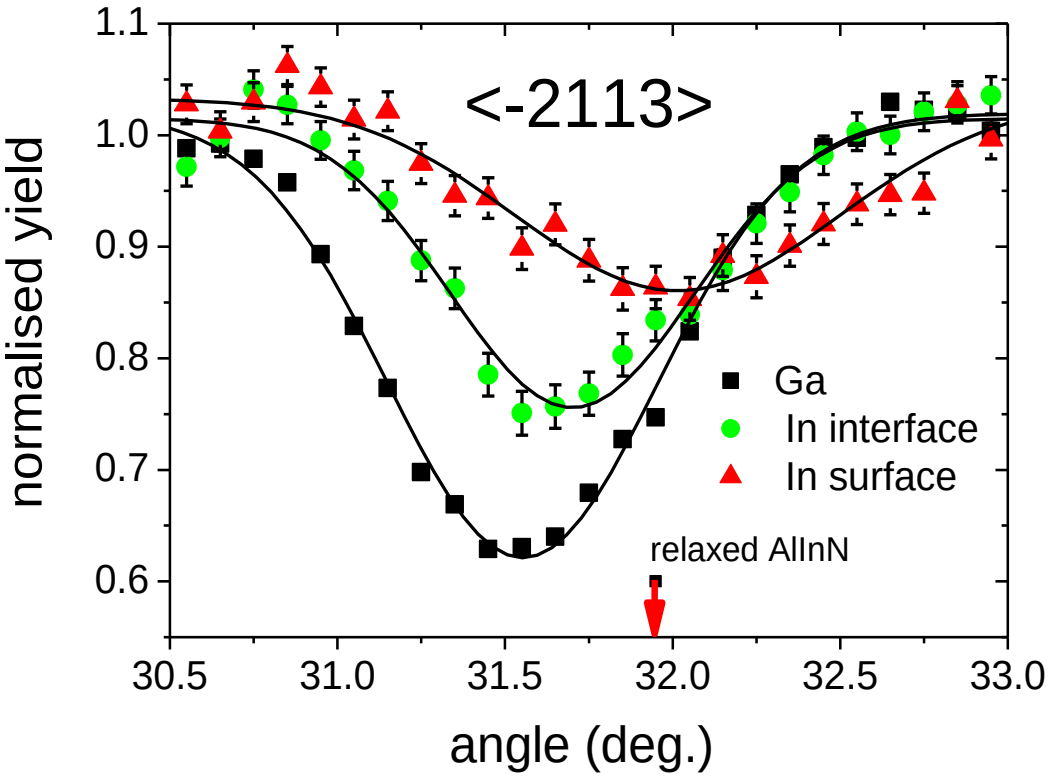
Lorenz et al. PRL 97 (2006) 85501
Lorenz et al. JCG 310 (2008) 4058

Strain Relaxation: Compressive Strain

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

Surface layer is relaxed
Deeper region under compressive strain

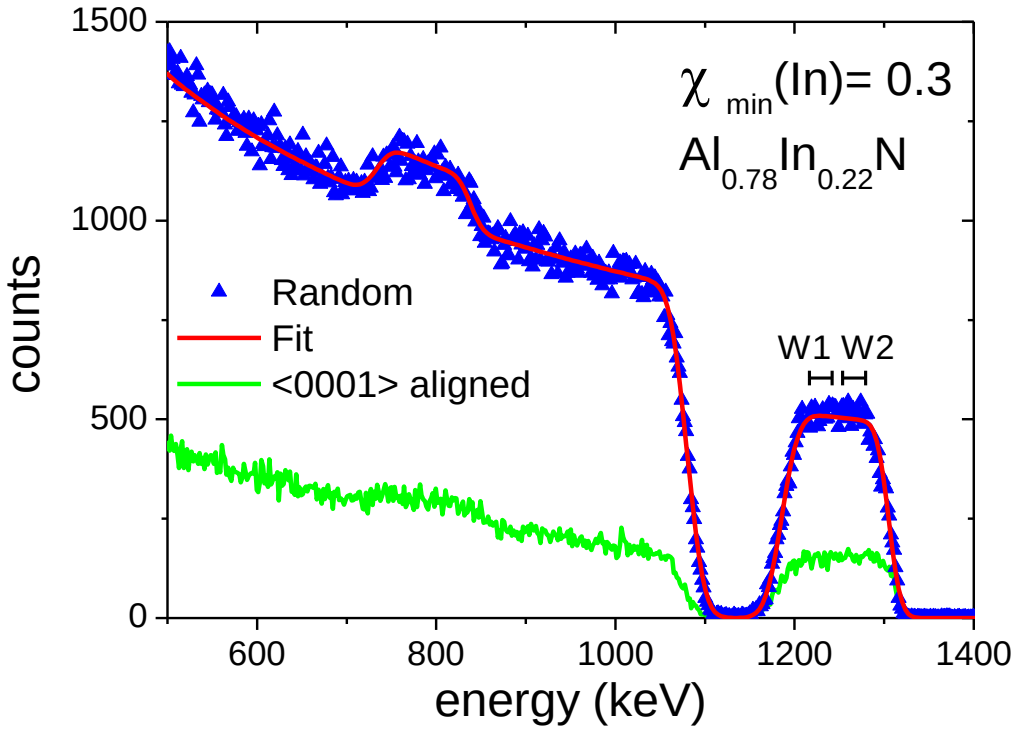




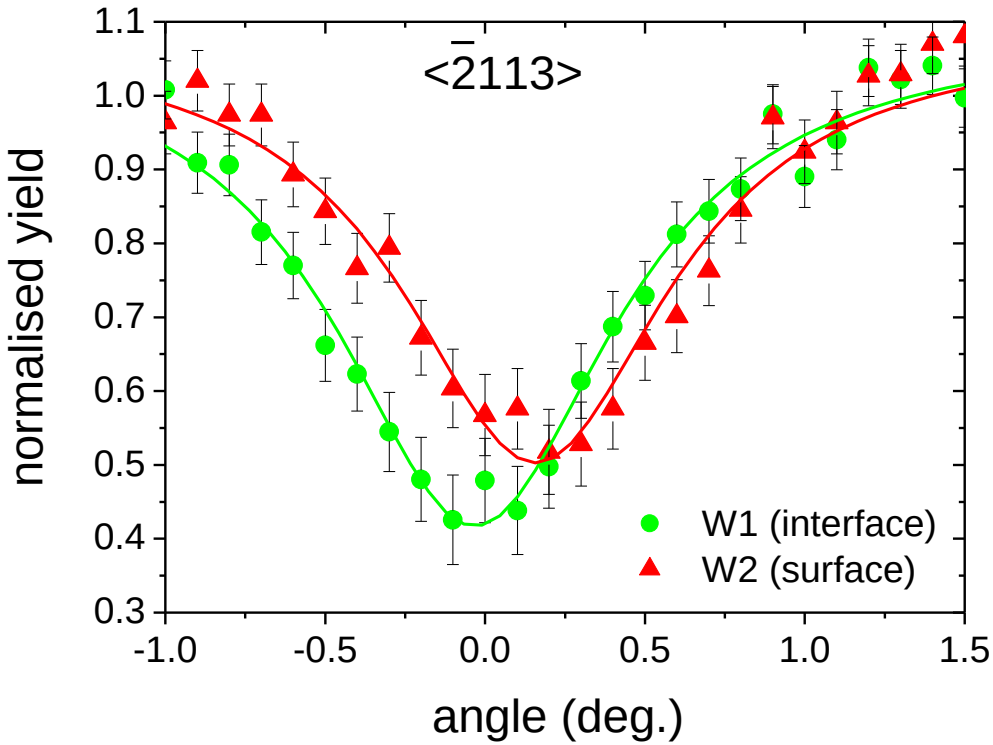
$\Rightarrow$ Relaxation via change of composition

Strain Relaxation: Compressive Strain

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



Relaxation towards the surface



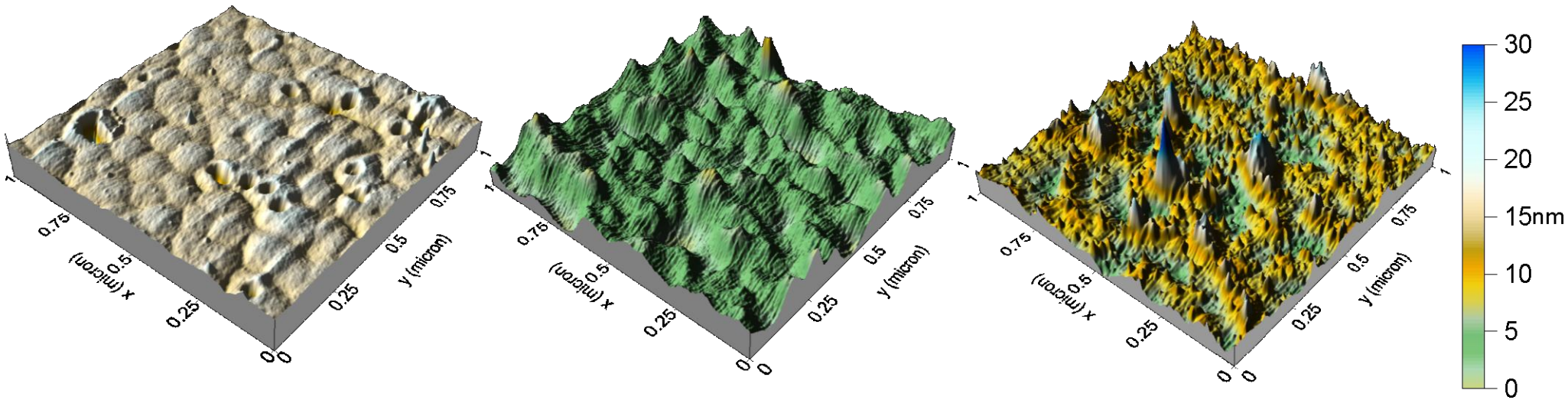
⇒ Relaxation via change of c/a ratio (constant composition)

Morphology Change

Pseudomorphic
x=.16

Partly relaxed
x=0.22

Relaxed
x=0.24→0.19



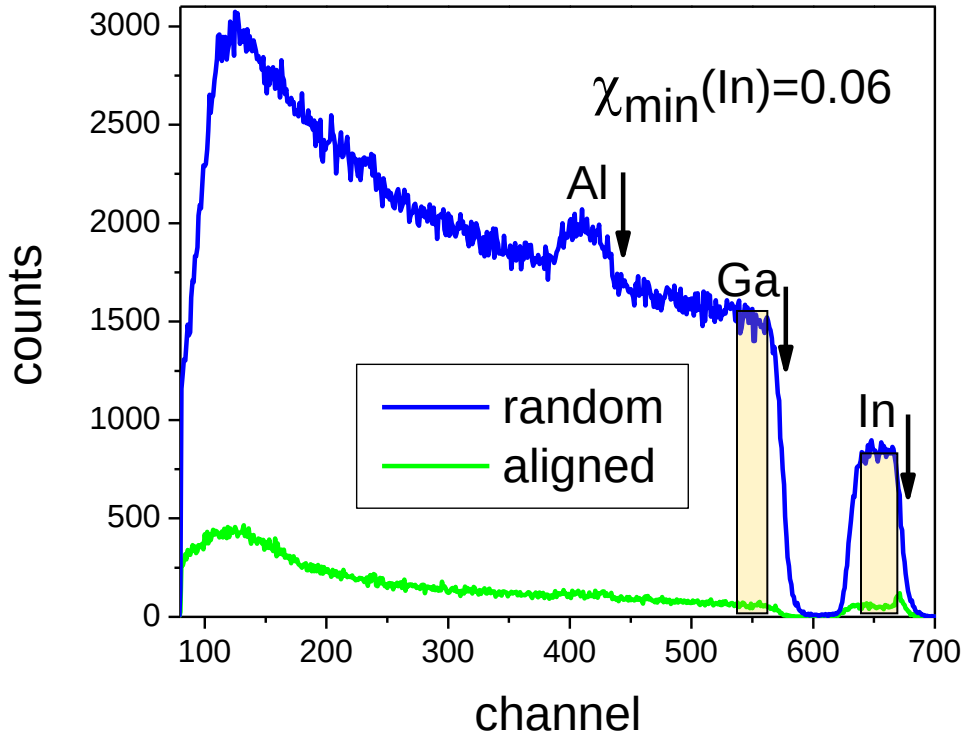
RMS=0.6 nm

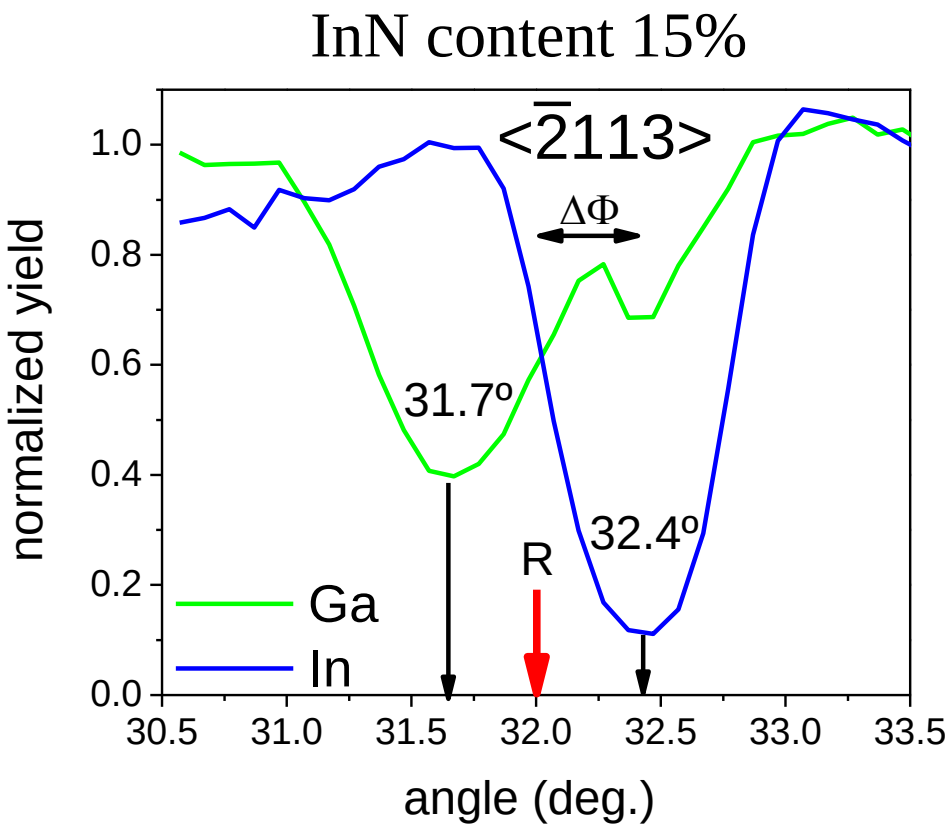
RMS=2.1 nm

RMS=6.2 nm

Roughening/3D growth

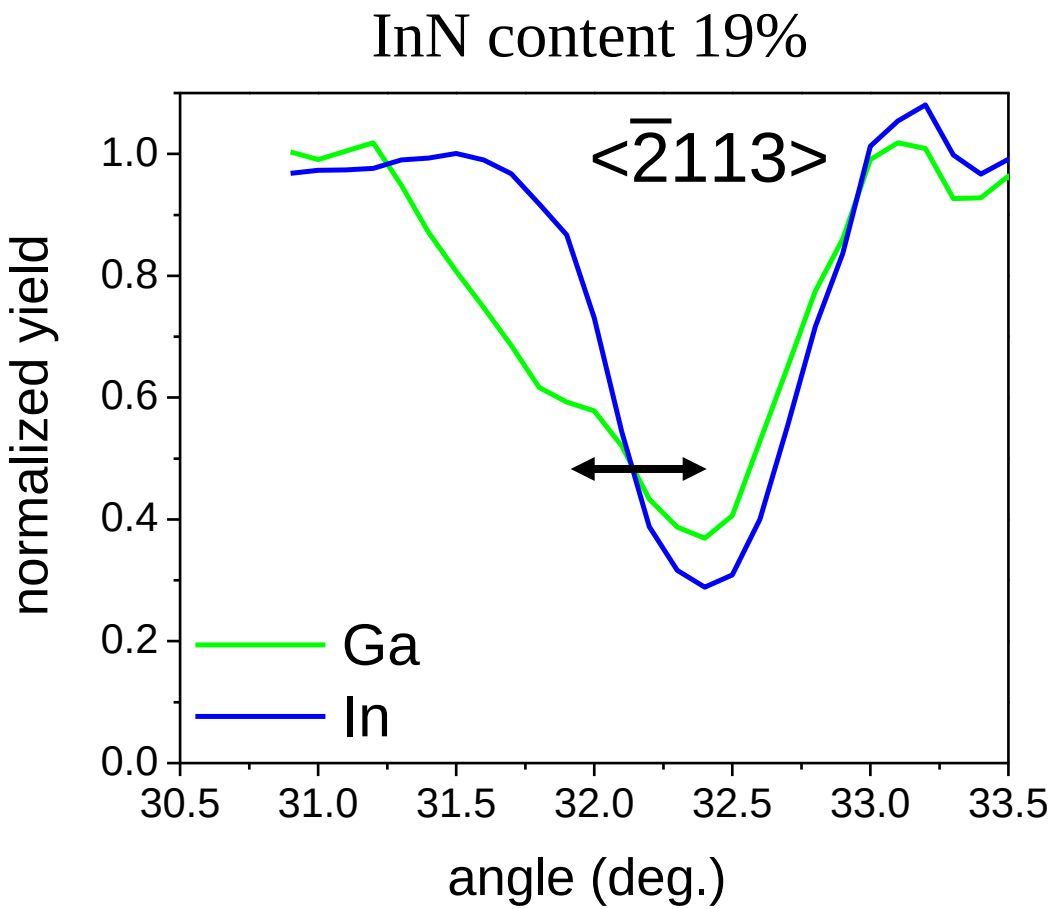
“Anomalous” features like double-dips





R: angle for relaxed AlInN
→ determined from Vegard´s law

Steering effects in the interface



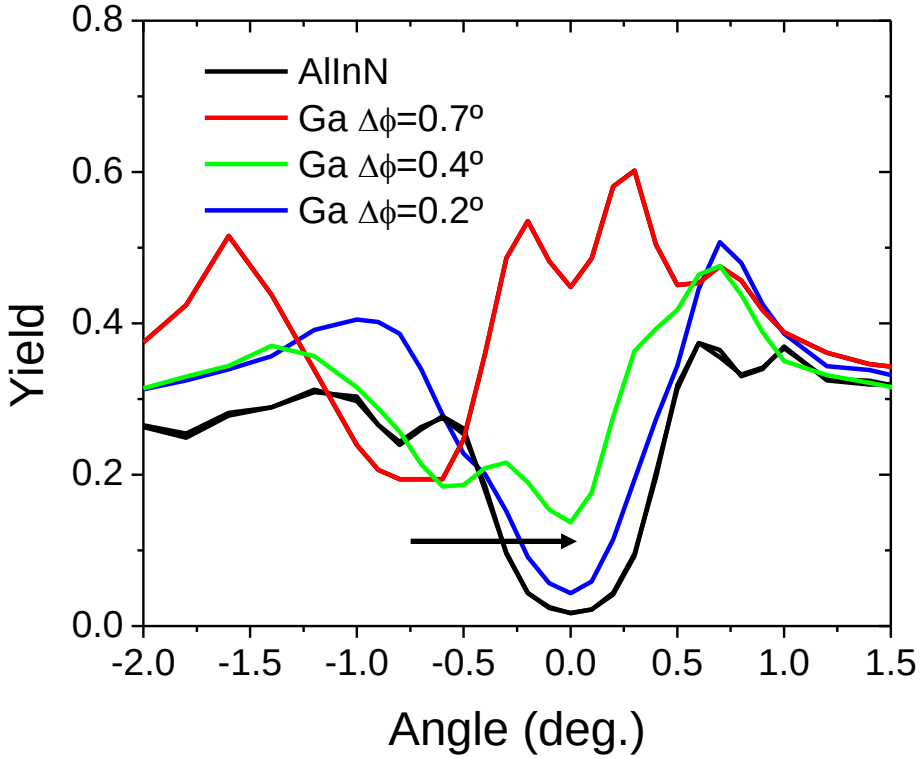
Angular scan of GaN substrate distorted when kink angle ≤ critical angle

→ α-energy

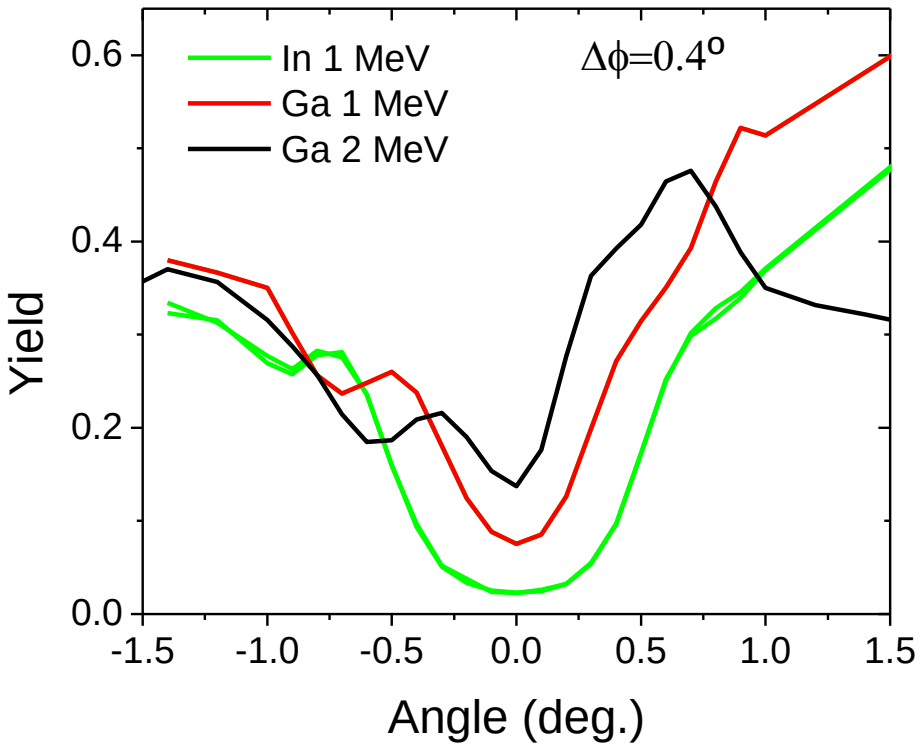
→ kink angle (InN content)

Steering effects: FLUX Simulations

Different kink angles



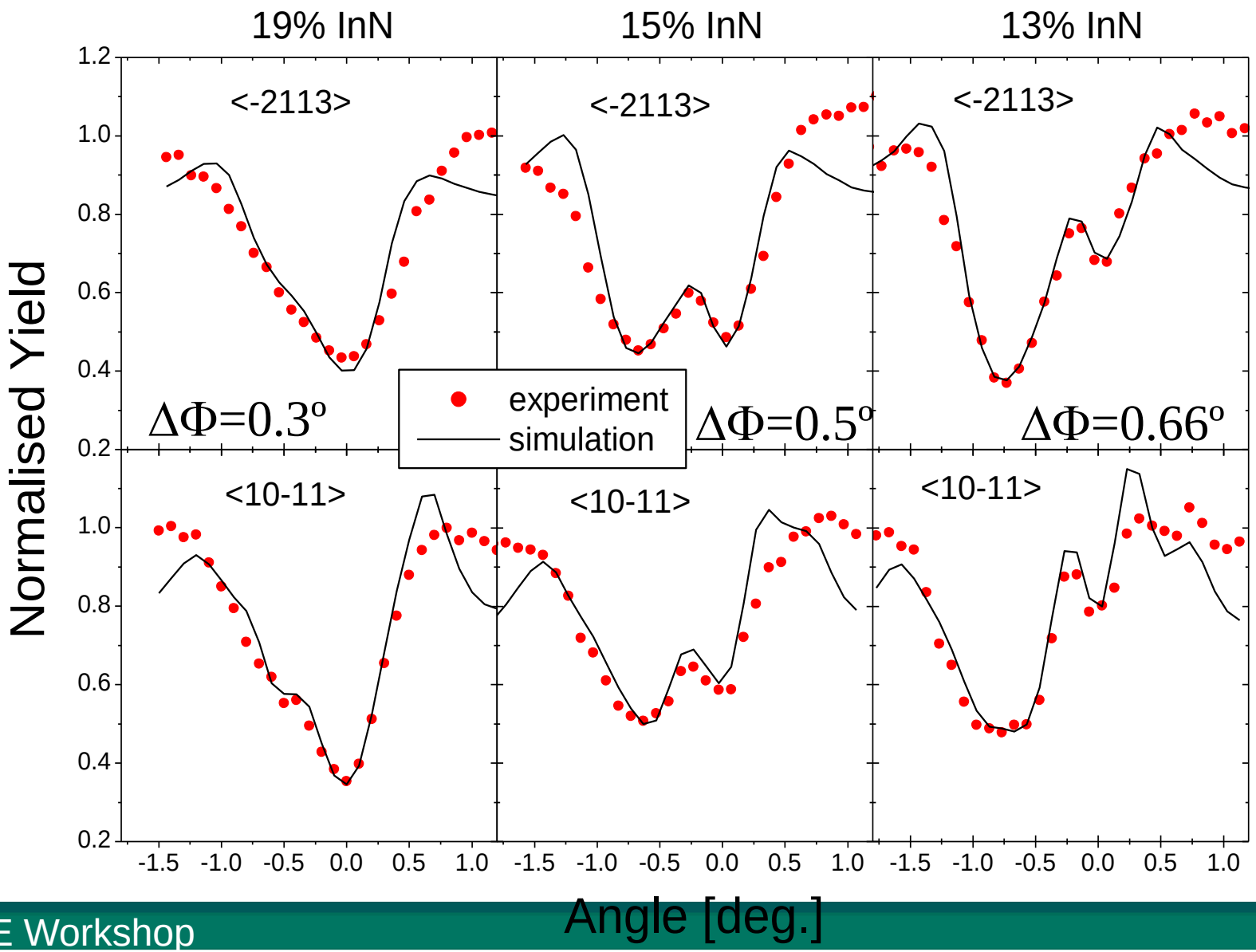
Different energies



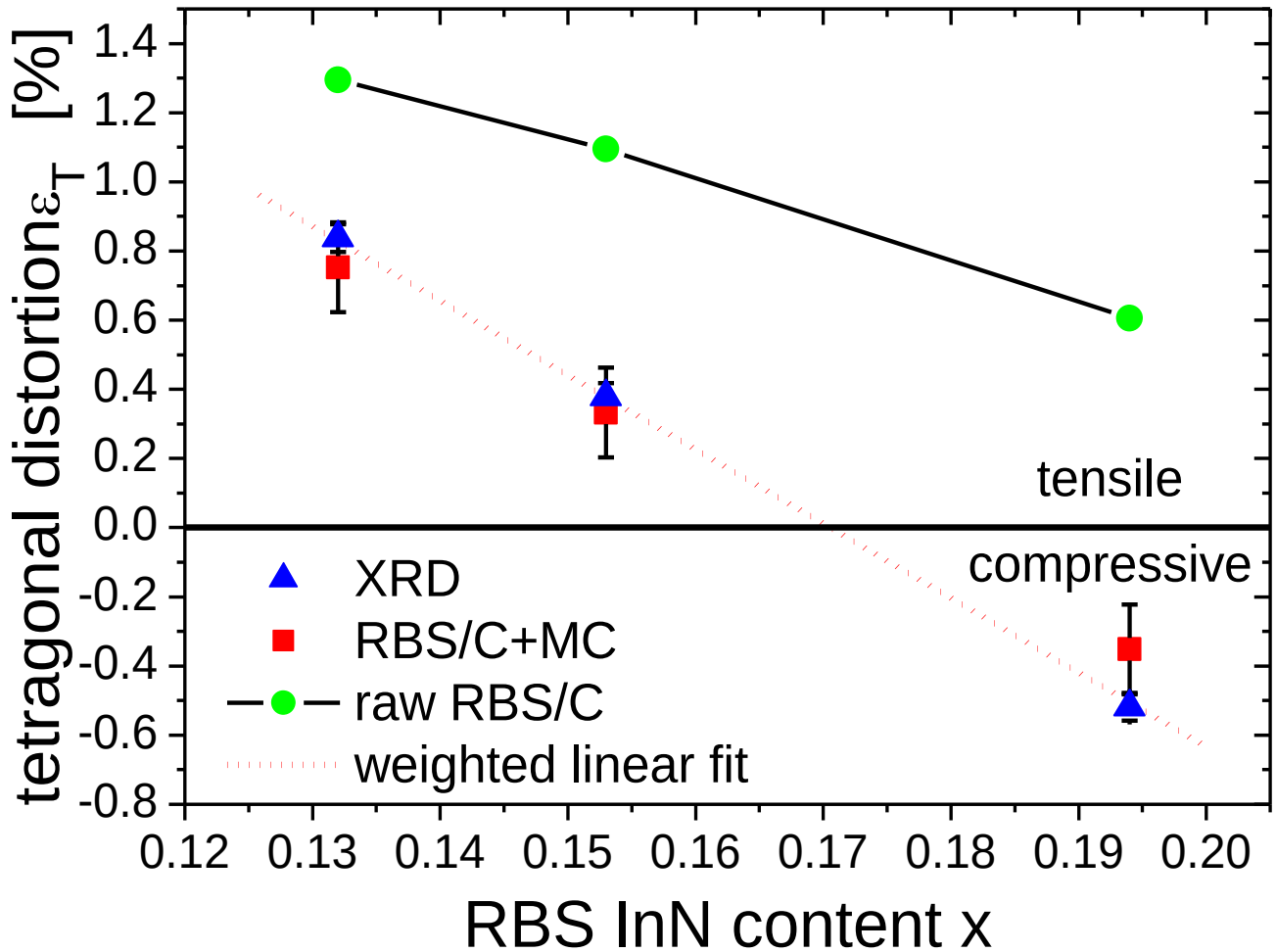
Redondo-Cubero, Lorenz et al. APL 95 (2009) 051921
Redondo-Cubero, Lorenz et al. JPD 42 (2009) 065420

→ Increasing beam energy
→ Comparison with simulations

GaN Scans and FLUX Simulations



Strain Analysis XRD - RBS



XRD

$$\varepsilon_\tau = \varepsilon^{\parallel} - \varepsilon^{\perp}$$

RBS

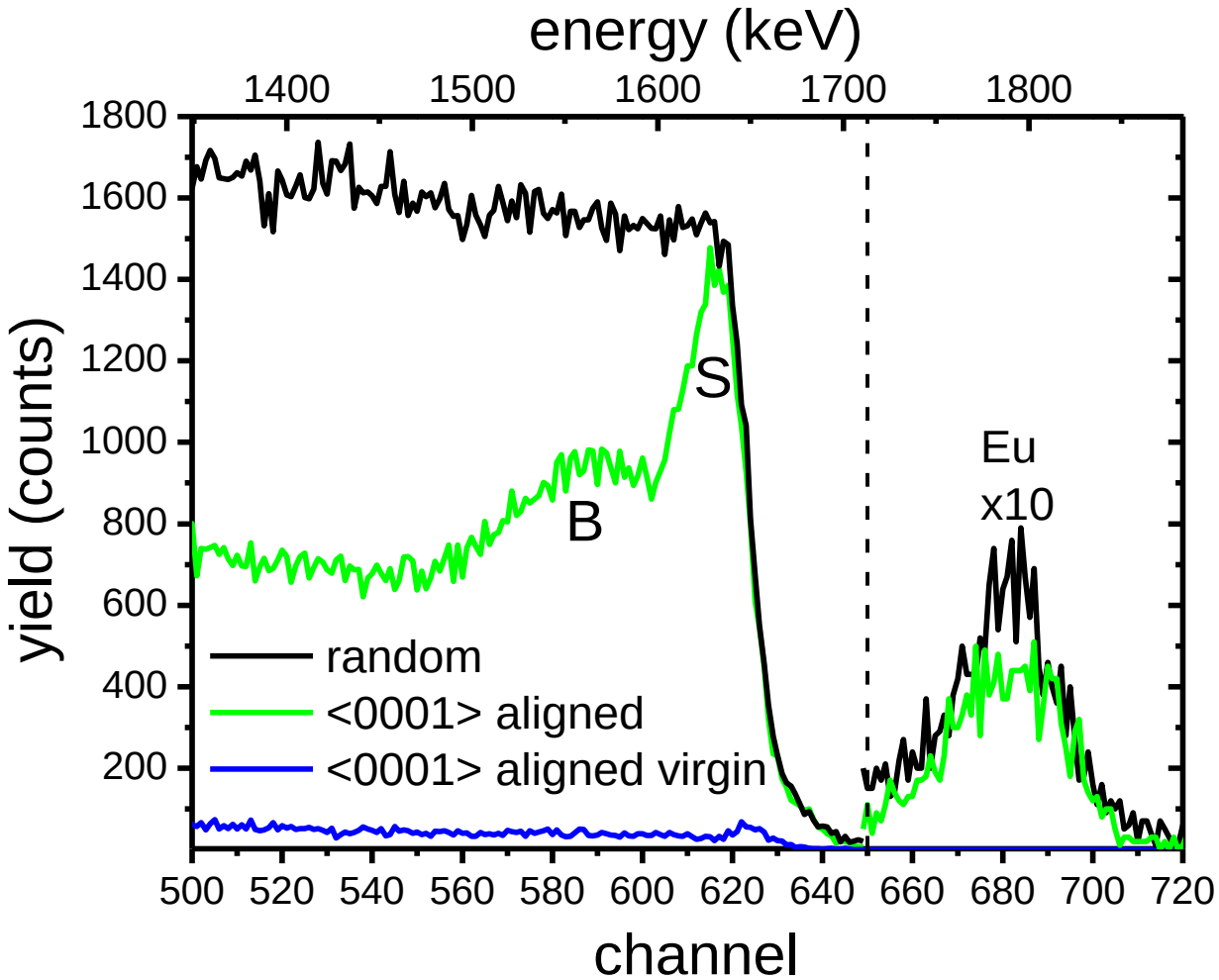
$$\varepsilon_\tau = \frac{\Delta\Phi}{\sin\Phi\cos\Phi}$$

Perfect Lattice matching for x=0.171

Lorenz et al. PRL 97 (2006) 85501

Implantation damage in GaN

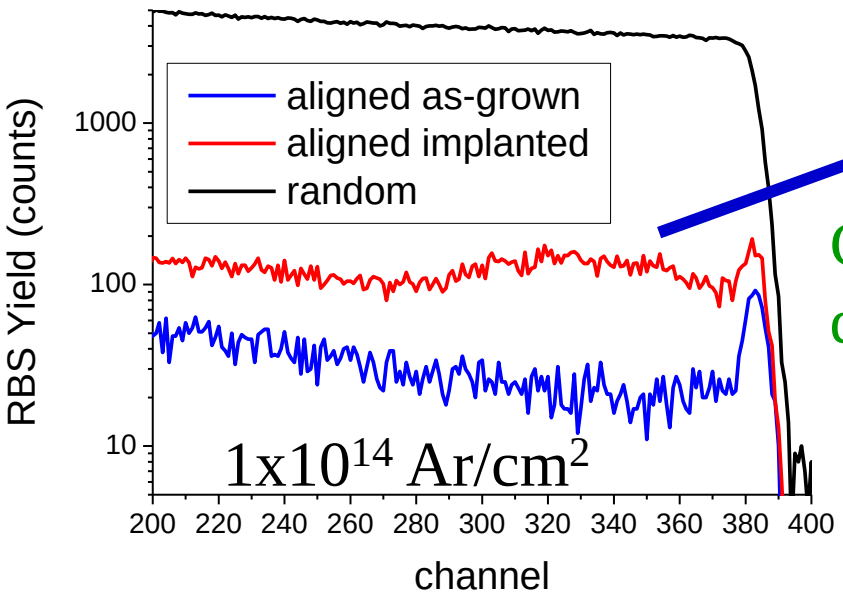
3×10^{15} at/cm^2 Eu implantation 300 keV at RT

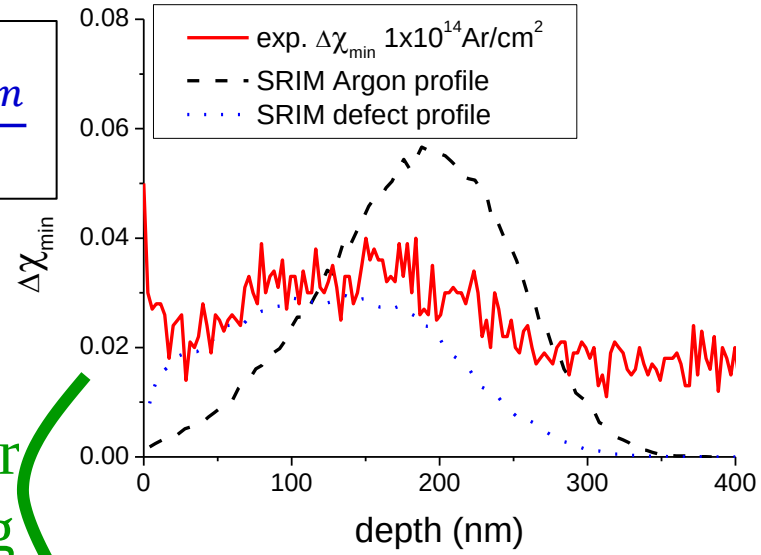


$\Rightarrow$ 2 damage regions (surface / bulk)

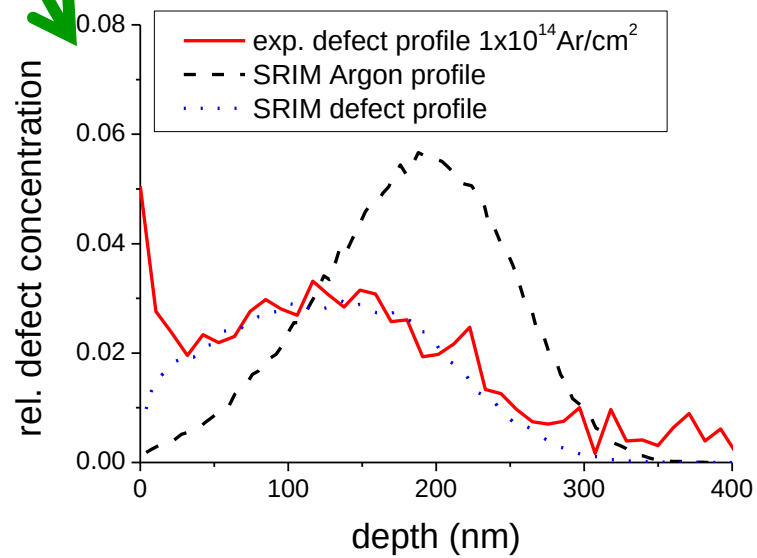
Implantation damage in GaN

$$\Delta\chi_{min} = \frac{Y^{aligned}_{as-implanted} - Y^{aligned}_{as-grown}}{Y^{random}}$$





Correction for dechannelling

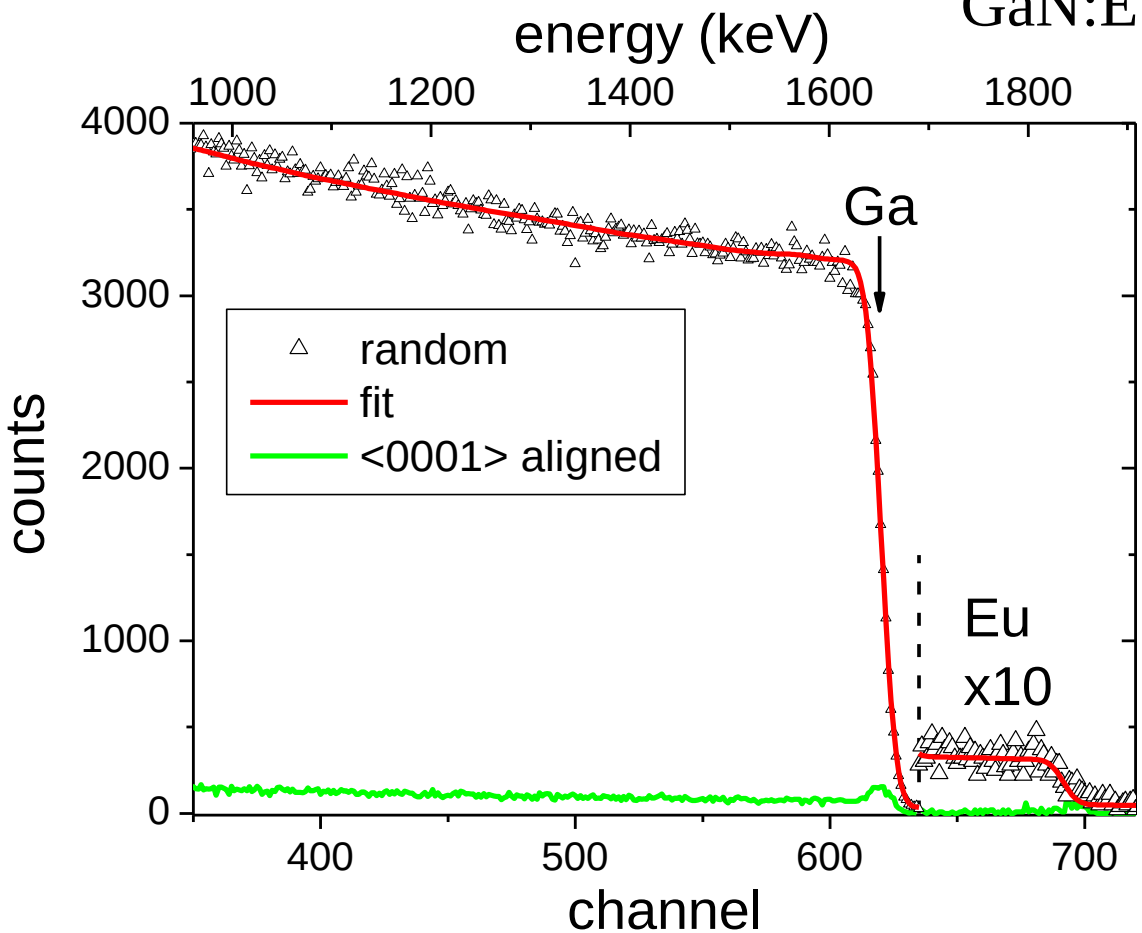


⇒ RBS/C aligned spectra need correction for dechannelling

(in this case using the DICADA program, Gärtner et al. NIMB **216** (1983) 275; **227** (2005) 522)

Lattice site location of Eu in GaN

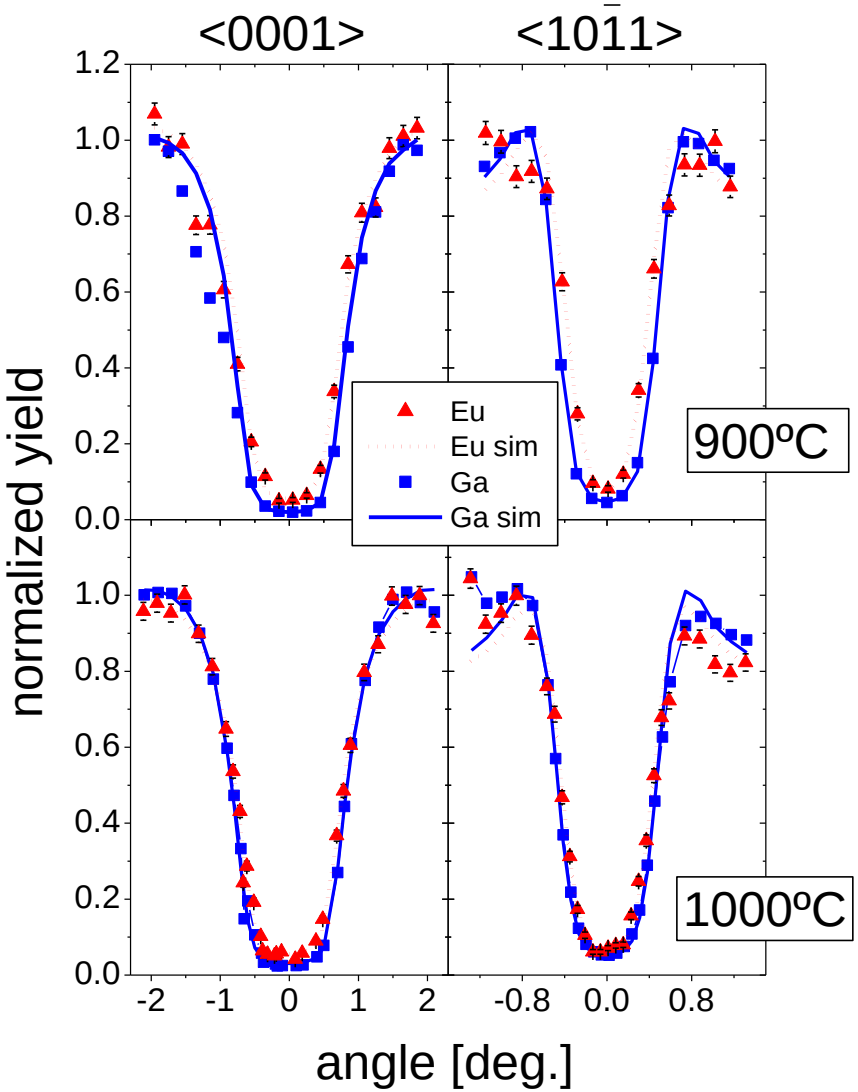
GaN:Eu grown by MOCVD at 1000ºC

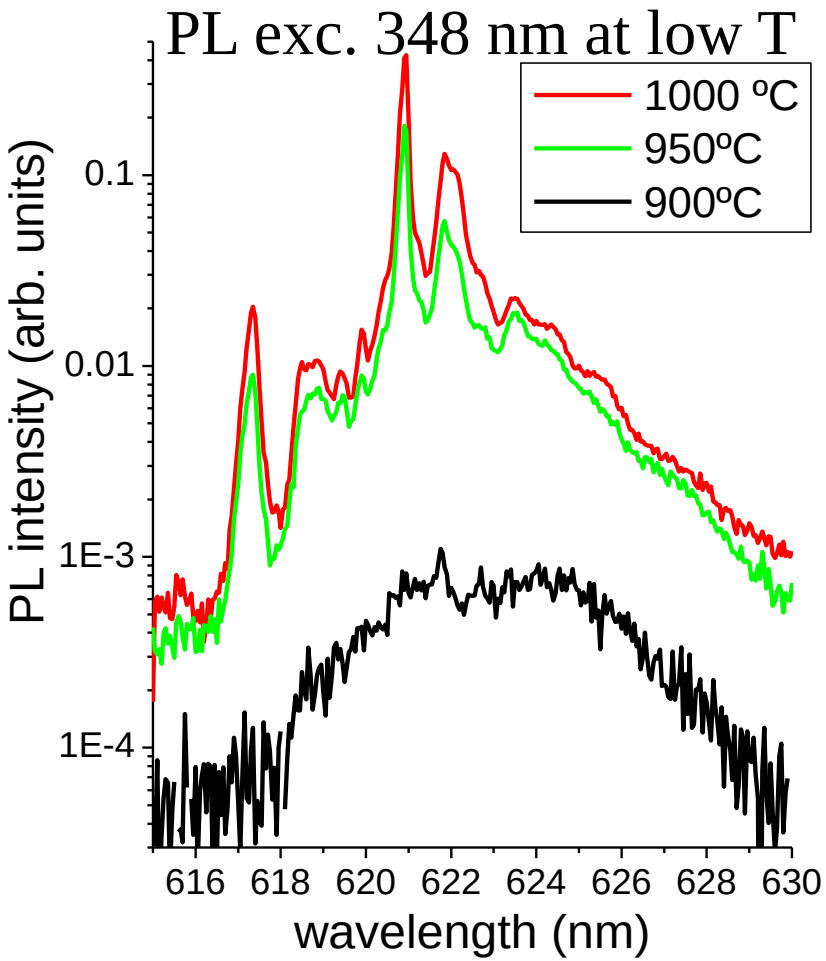


→ Homogeneous Eu distribution with depth ~0.1at%

→ Excellent crystal quality (Minimum yield <3%)

Lattice site location of Eu in GaN





→ Eu incorporated to ~100% on Ga-sites

→ Eu displaced (0.2Å) for sample grown at 900ºC

→ Eu clusters

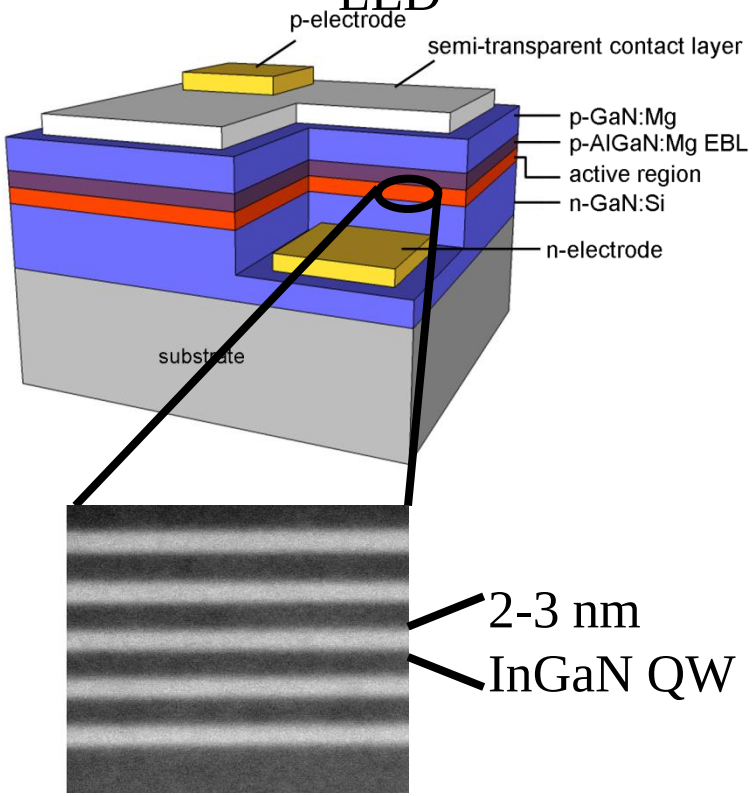
Lorenz et al. APL 97 (2010) 111911

Group-III Nitride Nanostructures

2D

InGaN/GaN quantum wells (QW)

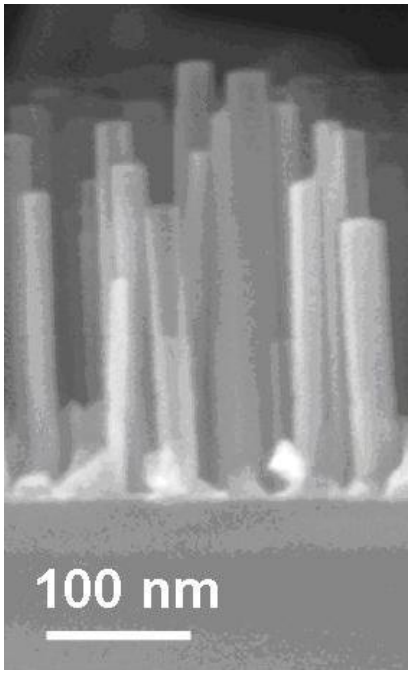
LED



1D

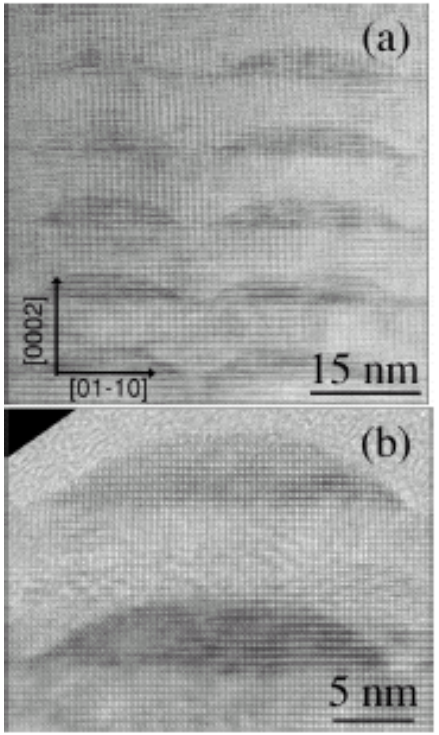
GaN nanowires (NW)

Nano-LEDs, sensors



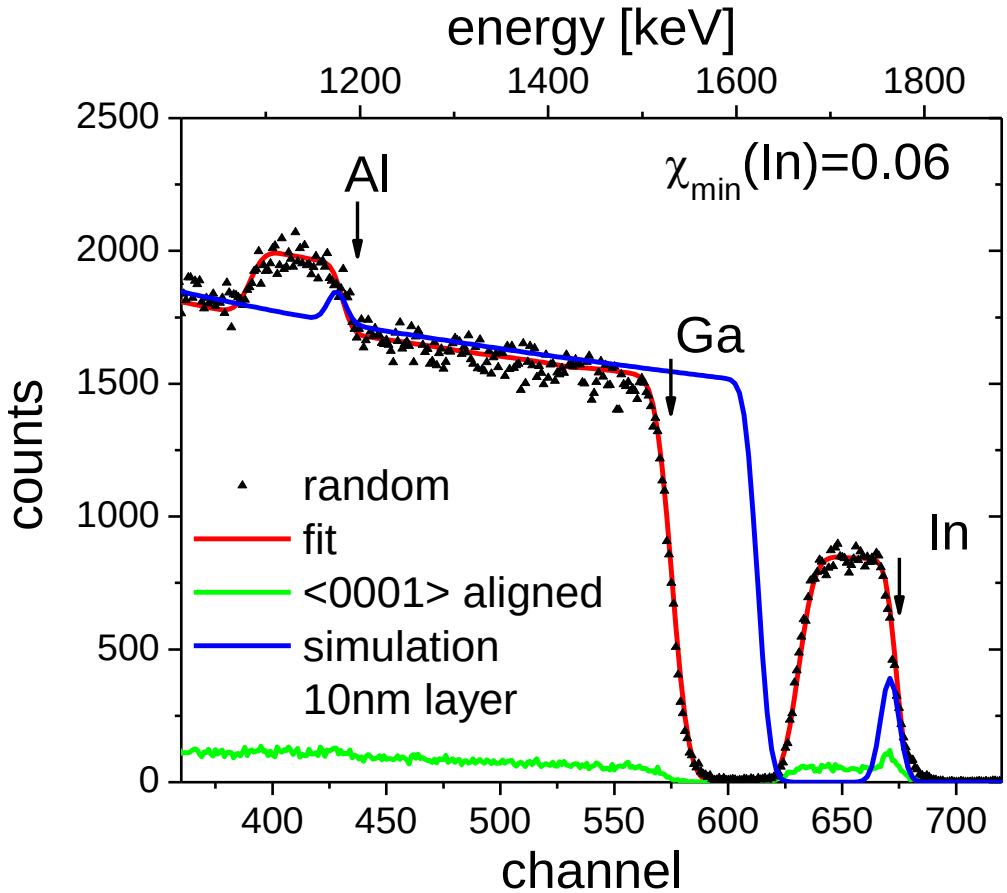
0D

GaN quantum dots (QD)



Problems when going to nano-scale

AlInN/GaN

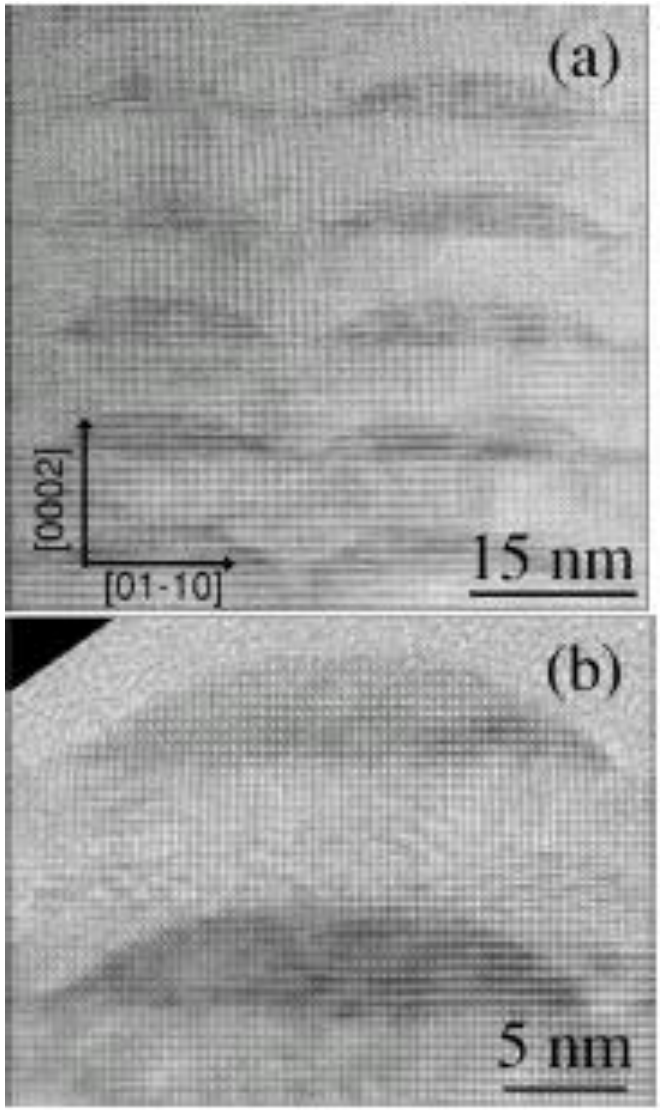


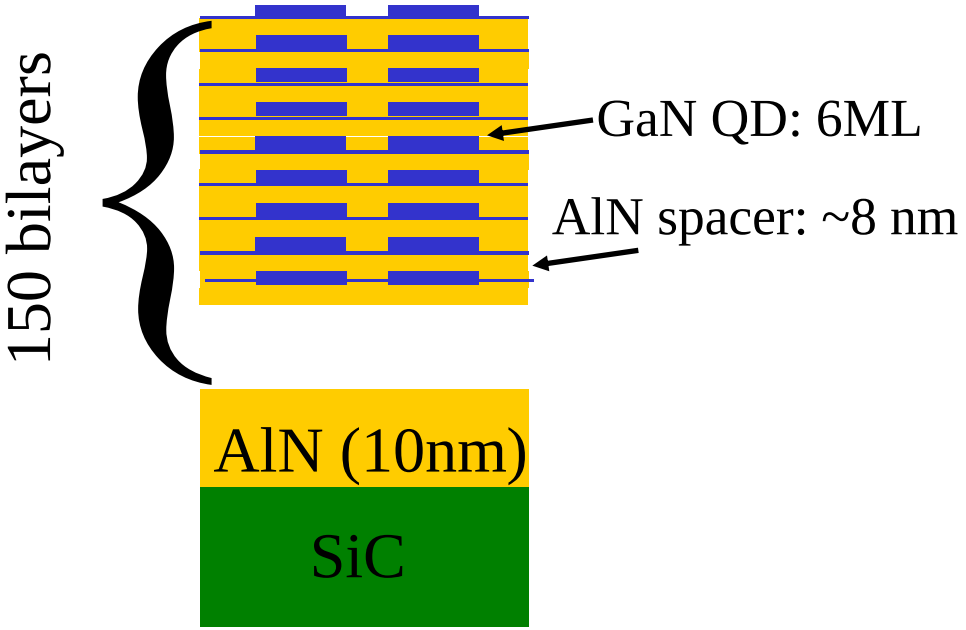
Limited depth resolution
in conventional RBS (~20nm)

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



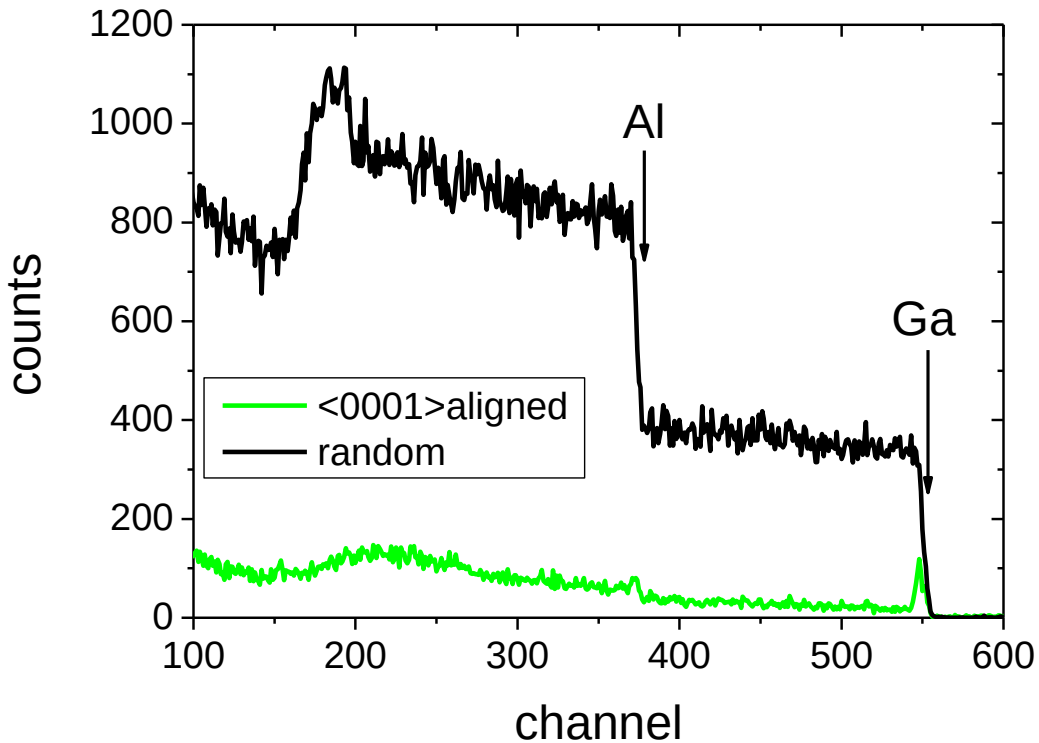


Grown by MBE using the Stranski-Krastanow growth mode

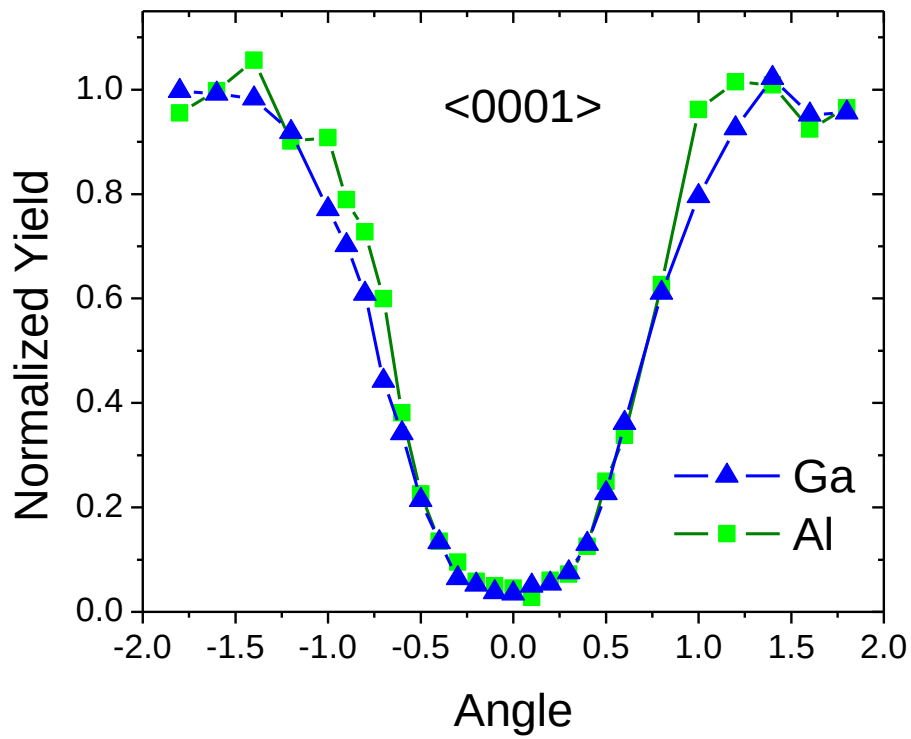
Chamard et al. Phys. Rev. B 69 (2004) 125327

RBS Normal Incidence

Random and <0001> aligned

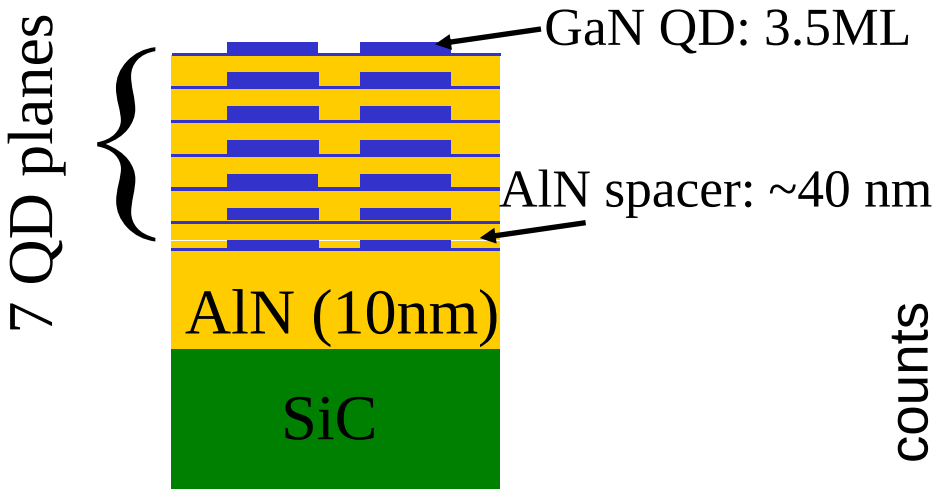


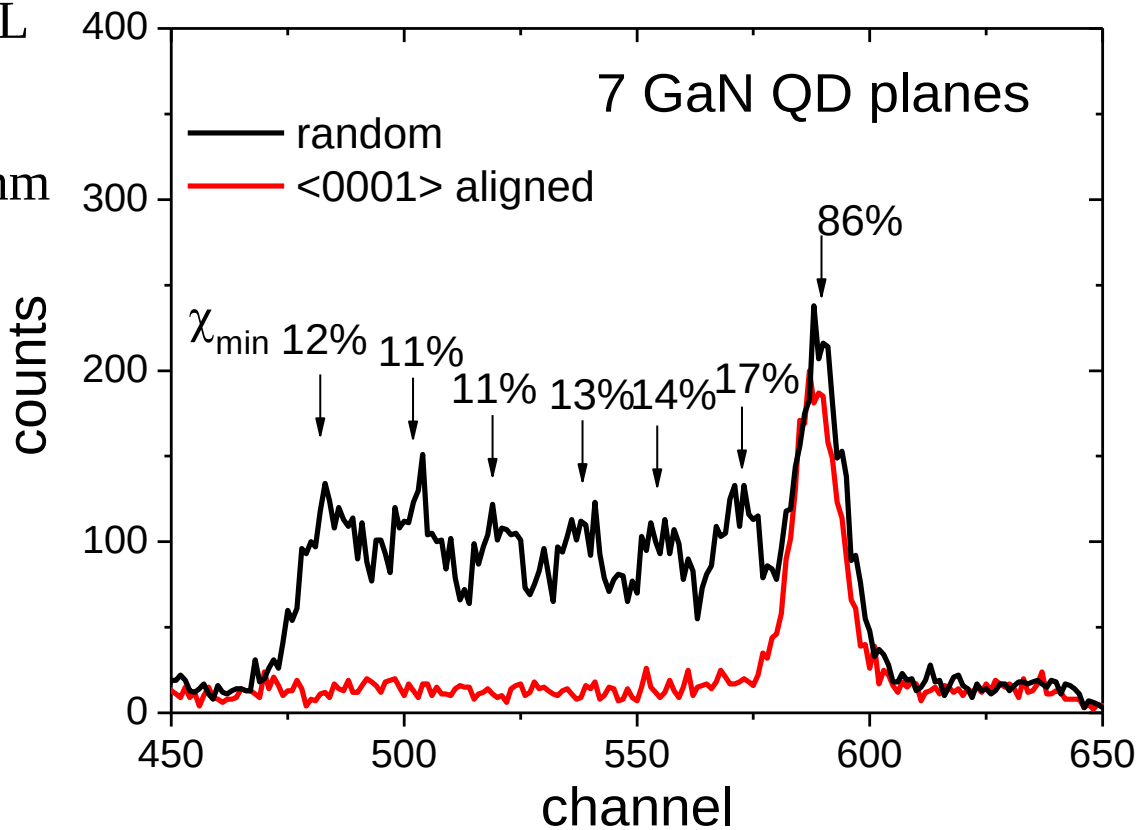
Scan across <0001>

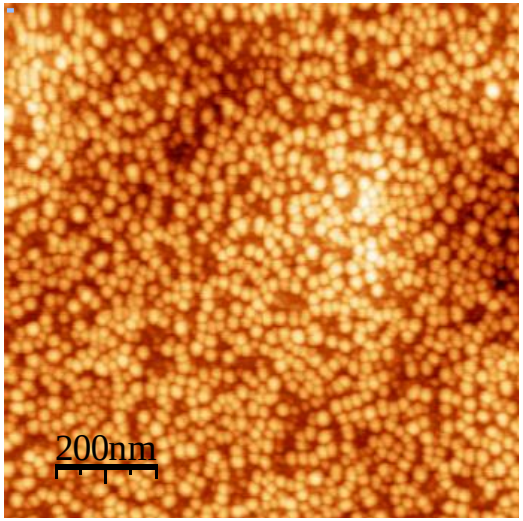


$\Rightarrow$ Excellent crystalline quality along c-axis χ_{min}=4%!

Crystal Quality of QDs







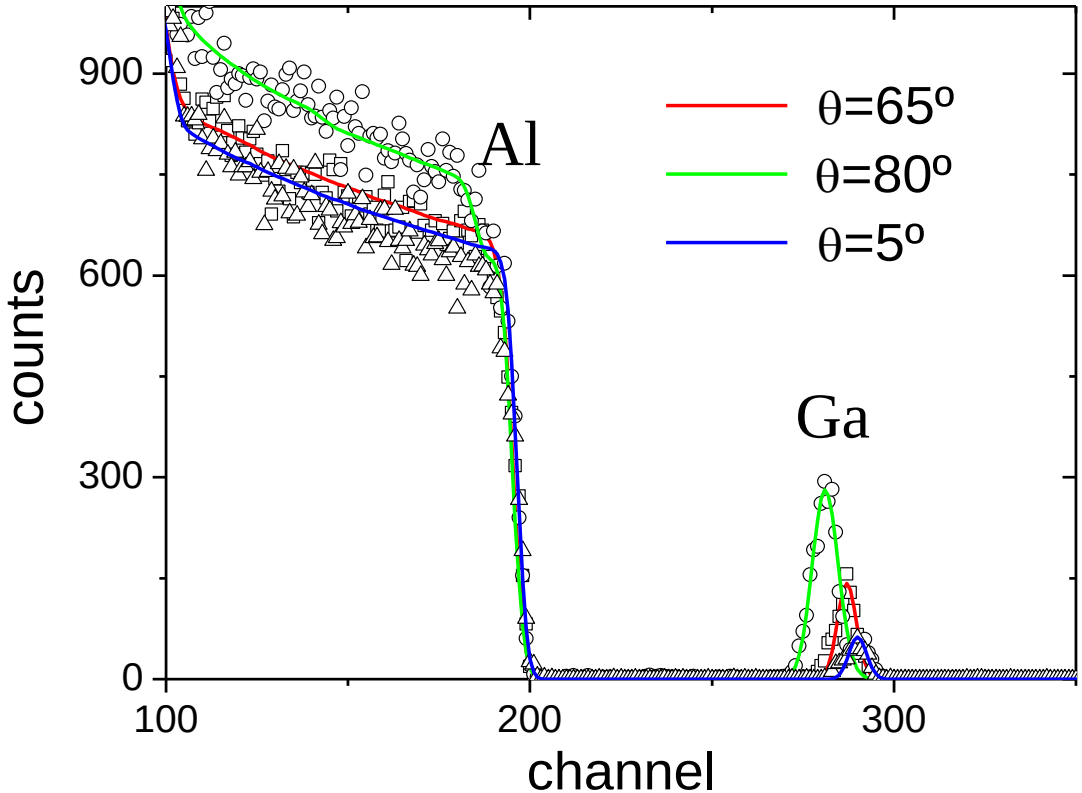
⇒ Crystal quality of each QD plane can be assessed and does not change with depth

⇒ QD at surface show reduced channelling probably due to strain relaxation and oxidation

Buried SQW / SQD-plane

10 nm
3.5 ML
26 nm

10 nm
3.5 ML
26 nm

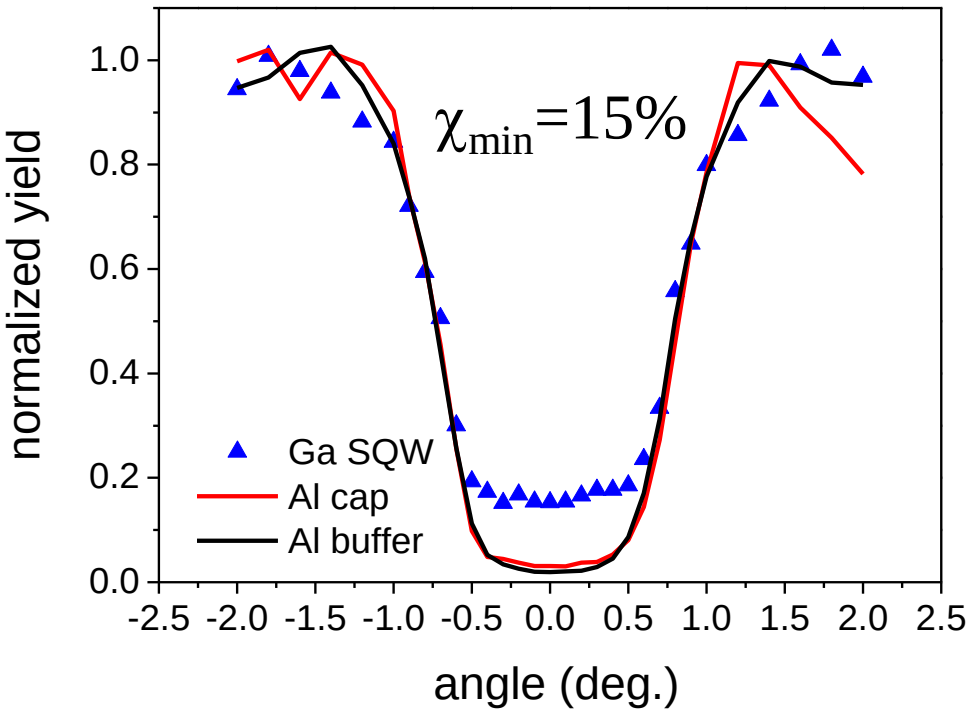


	RBS	XRR
AlN cap QD	8.9 (1.0) nm	9.4 nm
QD	2.6 nm (V_f=27%)	0.46 nm
AlN cap SQW	8.1(1.0) nm	8.8 nm
SQW	0.6 (1) nm	0.54 nm

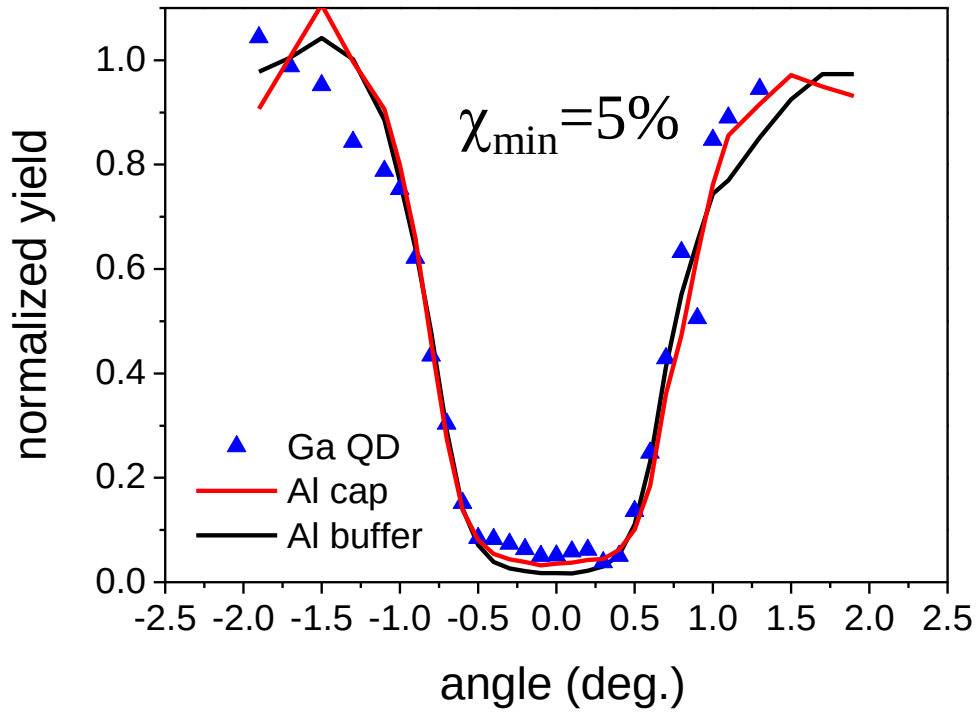
Quality Buried SQW / SQD-plane

<0001>

SQW



QD-plane

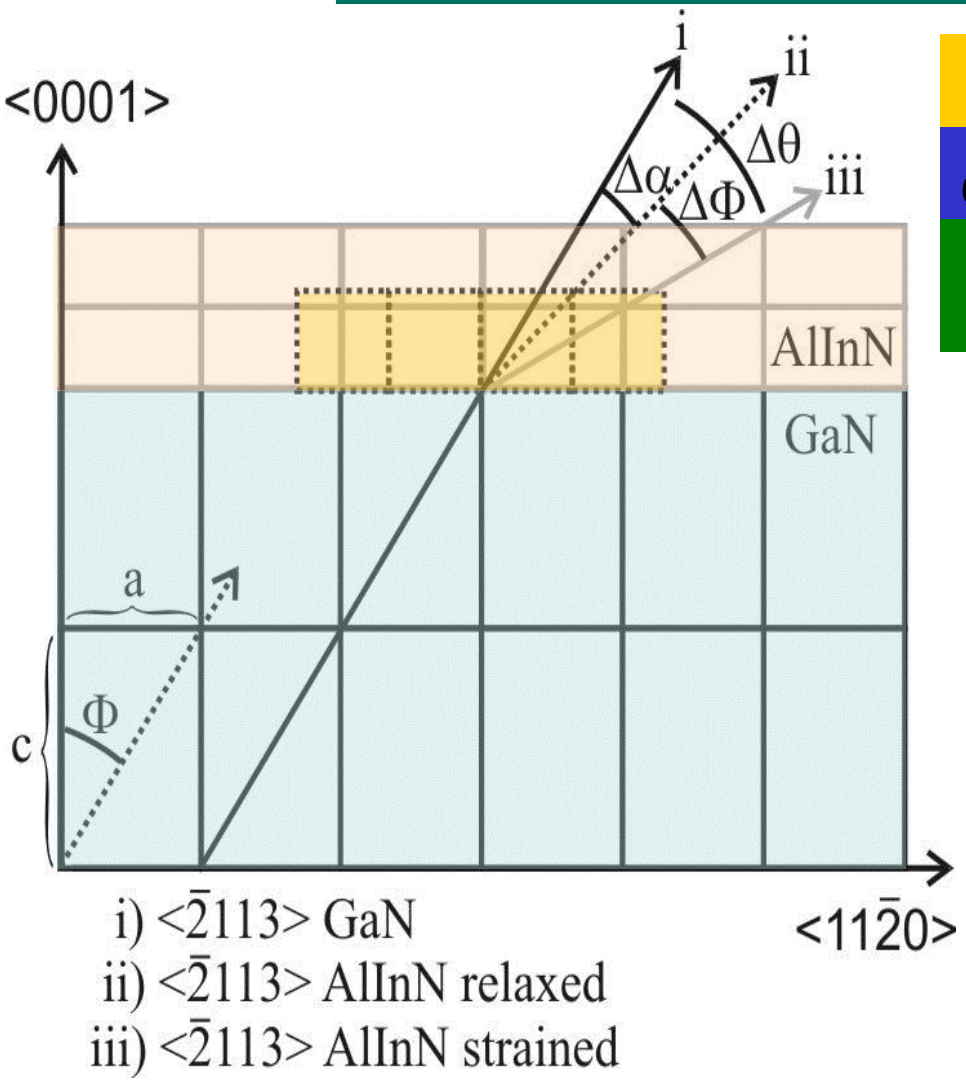


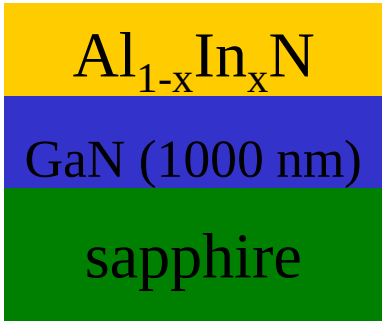
⇒ Crystal quality better in QD than in QW

⇒ Formation of misfit defects?

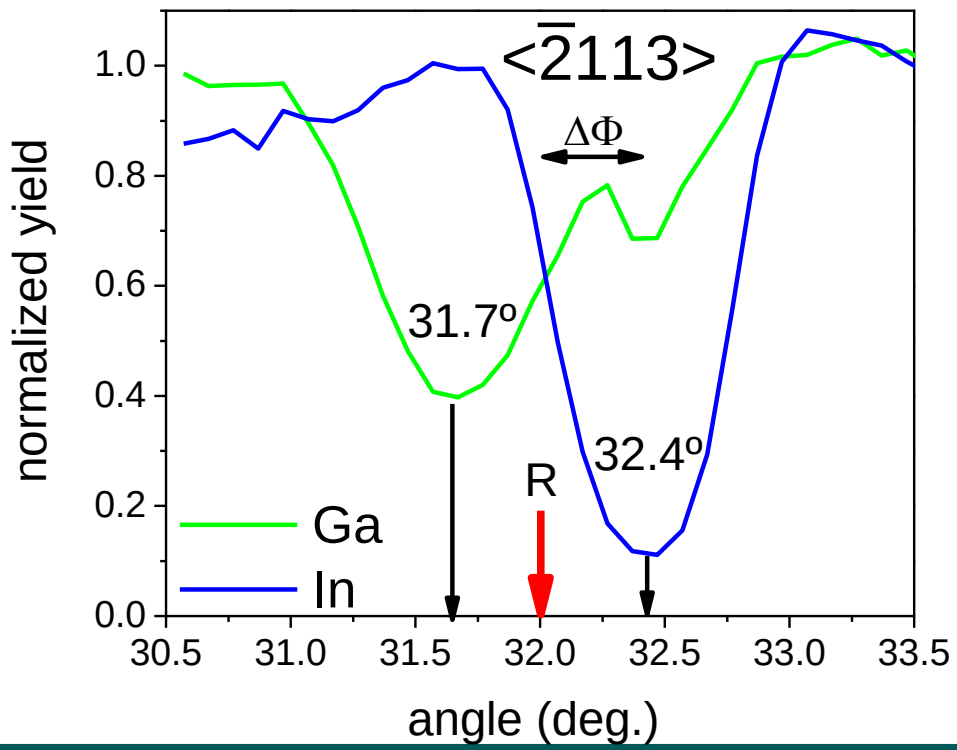
- misfit (GaN-AlN 2.5%) can lead to fomation of dislocations and stacking faults as evidenced by TEM analysis (Kandaswamy et al. JAP 106 (2009) 013526)

Strain measurement: thin film





$$\varepsilon_\tau = \frac{\Delta\Phi}{\sin\Phi\cos\Phi}$$

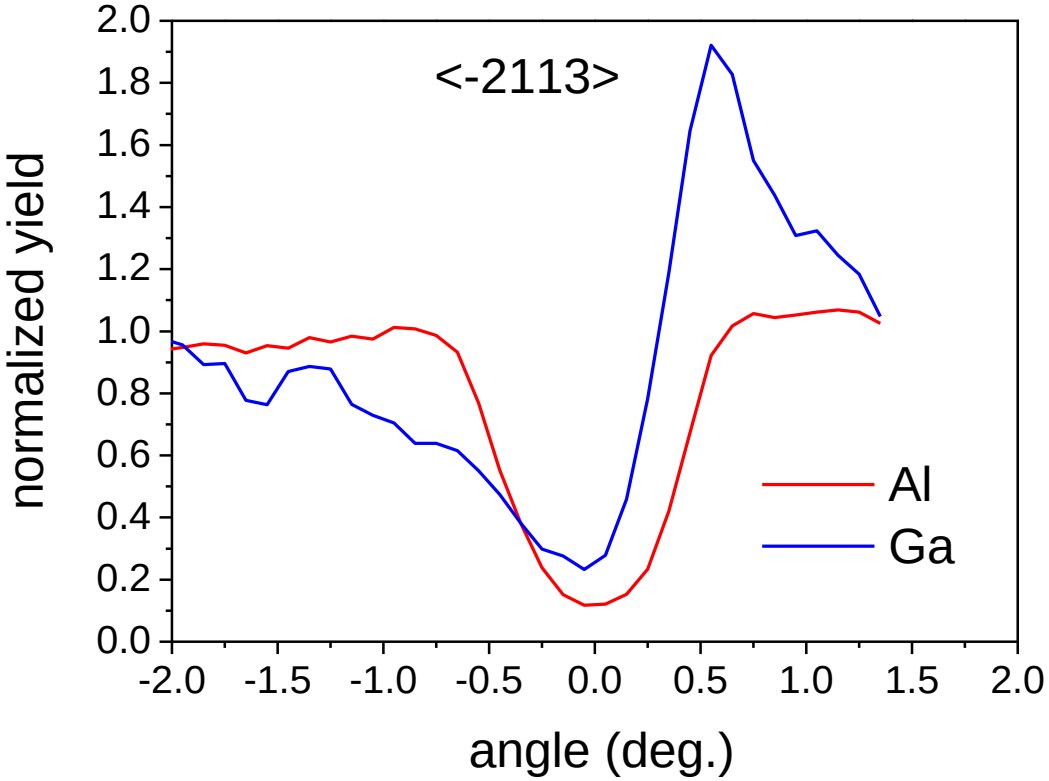


Lorenz et al. PRL 97 (2006) 85501; JCG 310 (2008) 4058

Problems when going to nano-scale

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

10 nm
3.5 ML
26 nm

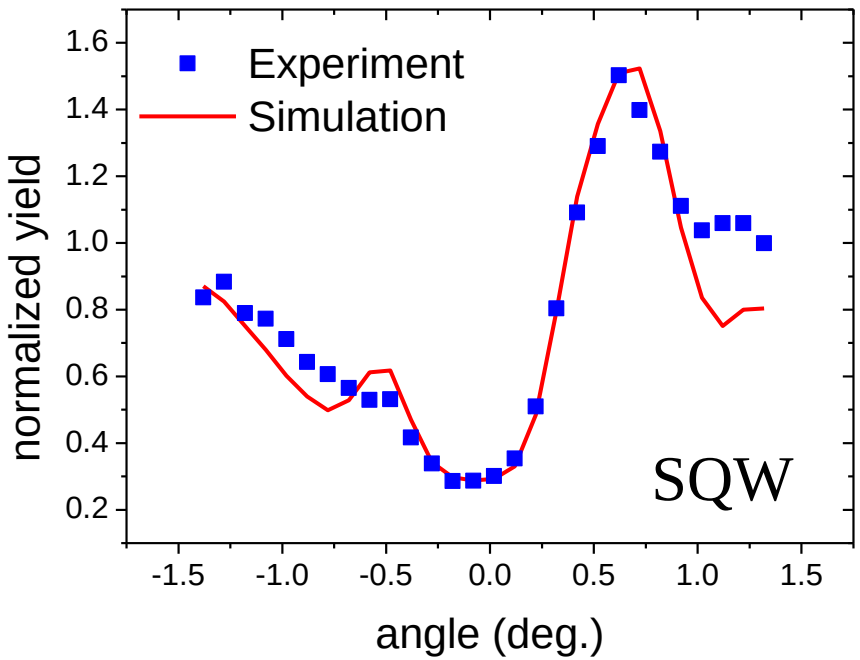


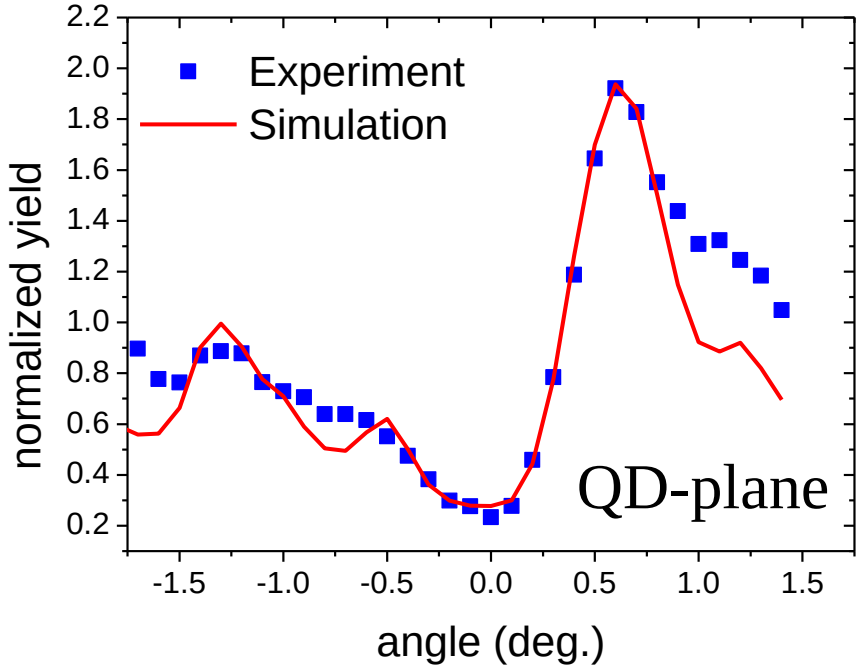
⇒ The GaN SQW is too thin to exhibit channelling effects on the beam

⇒ Ga-atoms act like an impurity

Scans do not shift but show asymmetries and flux peaking

Strain in Buried SQW / SQD-plane





0.9 nm QW ⇒ $\Delta\theta$=0.14º ⇒ ε_T=-3.9%

0.6 nm QW ⇒ $\Delta\theta$=0.22º ⇒ ε_T= -7%

ε_T (fully strained)=-3.6%

⇒ QD partly relaxed but error in current data anlysis is extremely high

0.9 nm QD ⇒ $\Delta\theta$=0.12º⇒ ε_T= -3.1%

1.7 nm QD ⇒ $\Delta\theta$=0.7º ⇒ ε_T= -1.6%

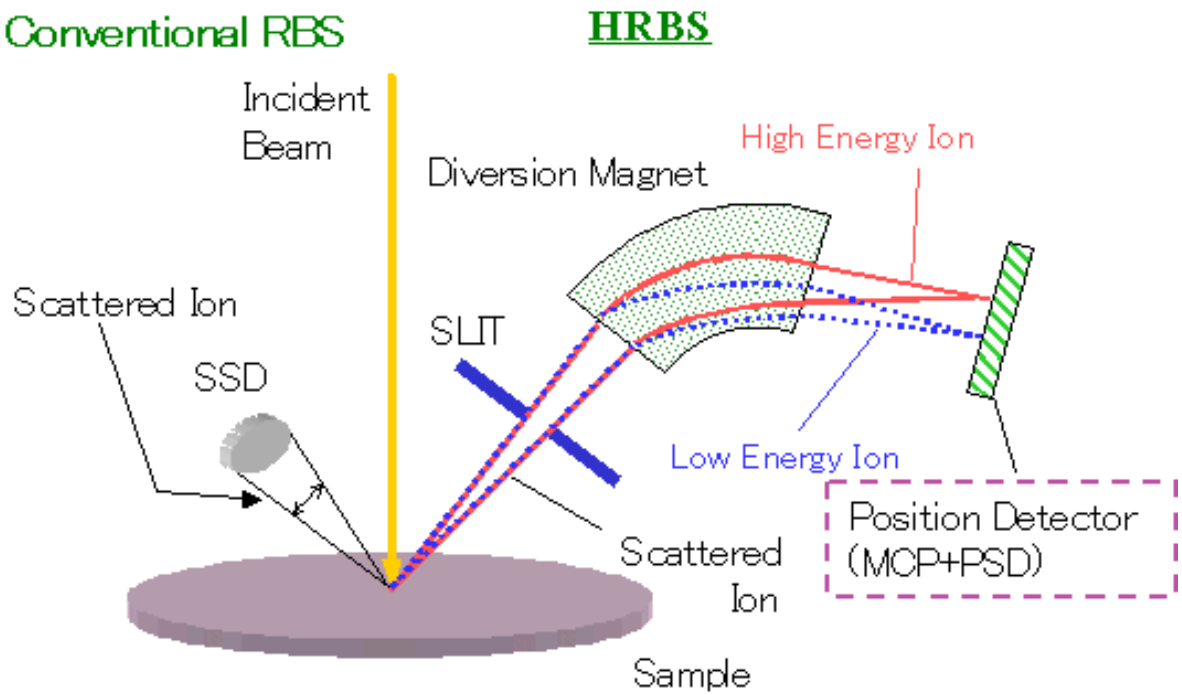
2.6 nm QD ⇒ $\Delta\theta$=0.5º ⇒ ε_T= -0.4%

ε_T (Raman, XRD)= -2.4%
(Cros et al. PRB 76 (2007) 165403)

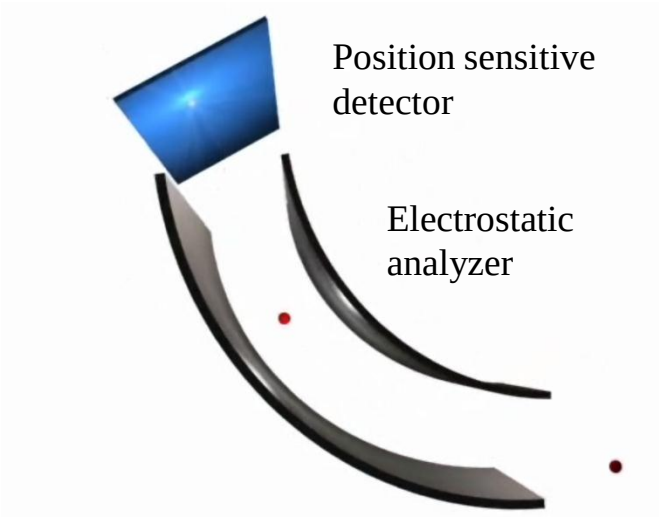
⇒ MC simulations need to include sample imperfections and QD

High resolution RBS or MEIS

	RBS	HR-RBS / MEIS
Energy	~ 1-5 MeV (α, p)	~ 50-500 keV (α, p)
Detector system	Si surface barrier detector	Electrostatic analyser or magnetic spectrometer:
Resolution of detector system	~ 15 keV	< 1 keV
Depth resolution	~10 nm	< 1 nm
Probing depth	~1 μm	~20 nm

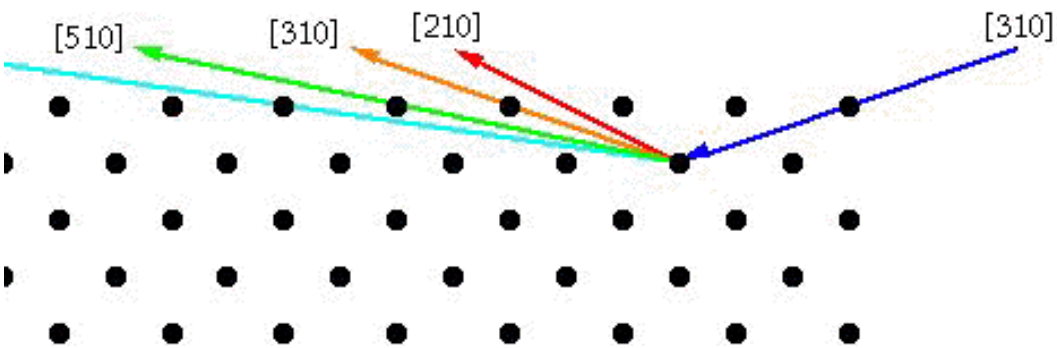


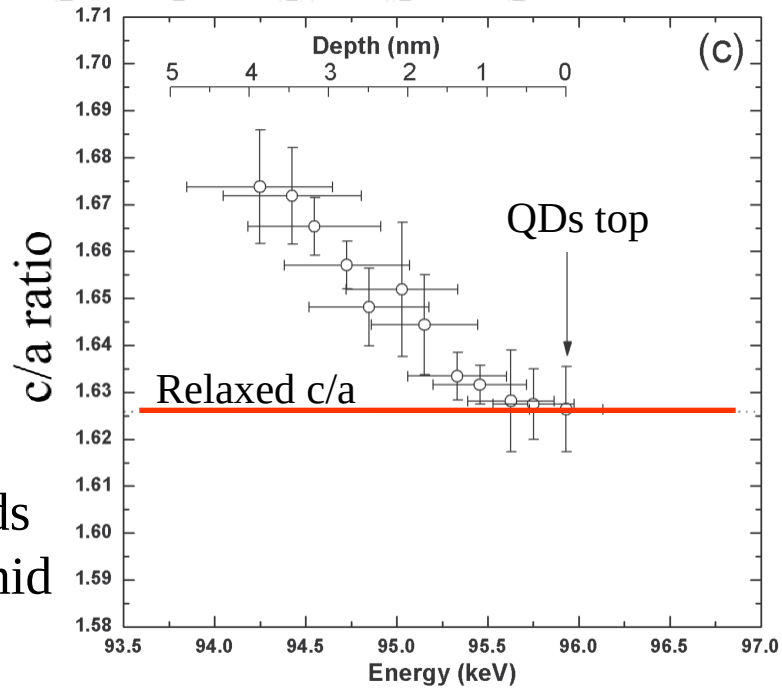
MEIS

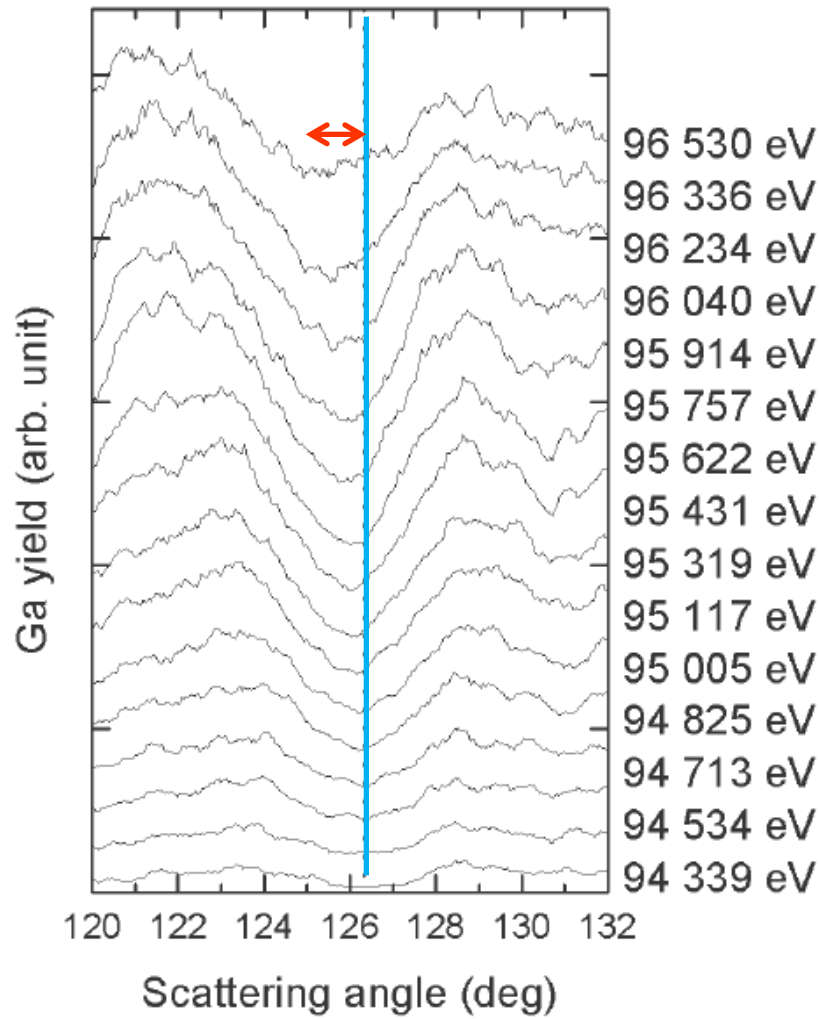


MEIS: Strain distribution in GaN QDs

Blocking



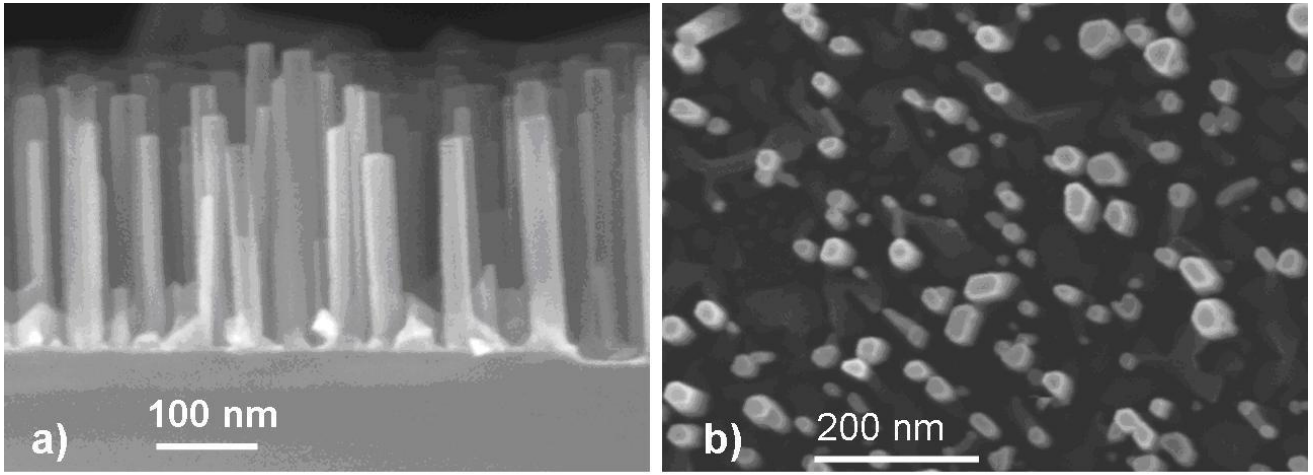




⇒ QD relax towards the top of the pyramid

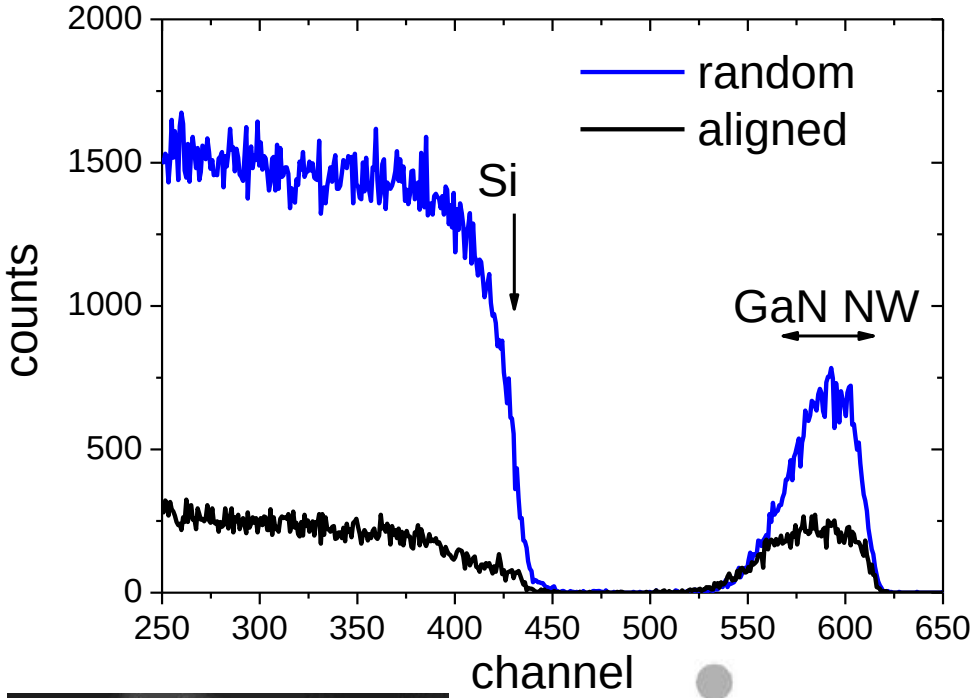
Jalabert et al. PRB 72 (2005) 115301

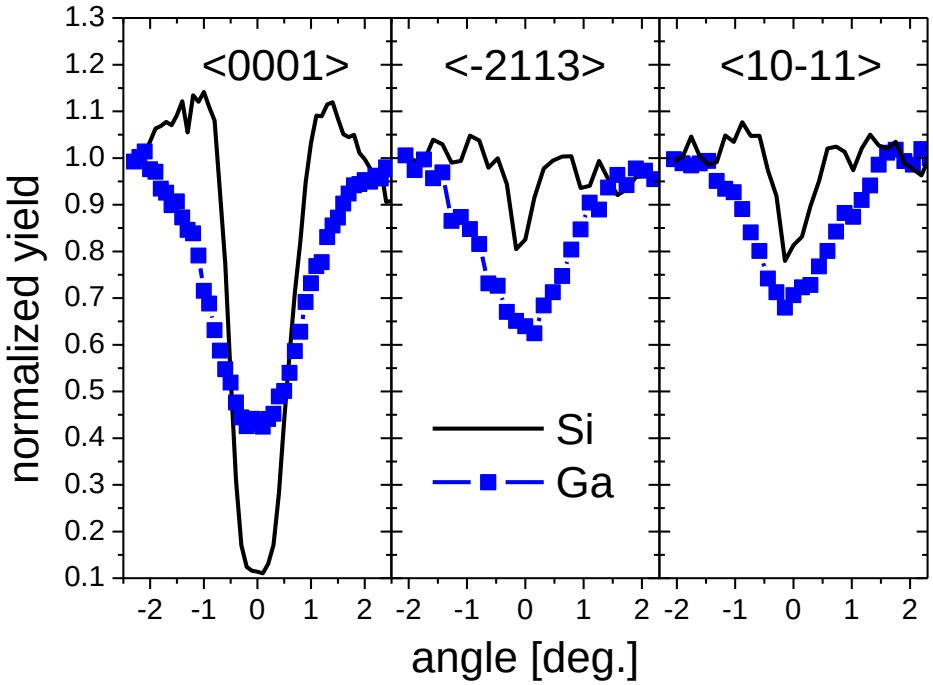
RBS/C on nanowires?

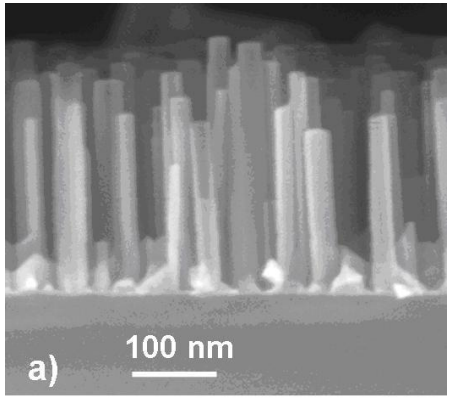


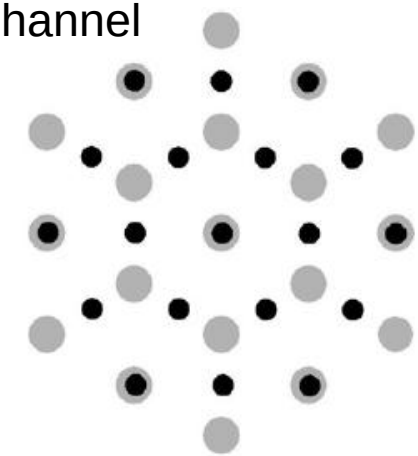
- Vertically aligned NW grown by MBE on 111 Si

Alignment of Nanowires









Si

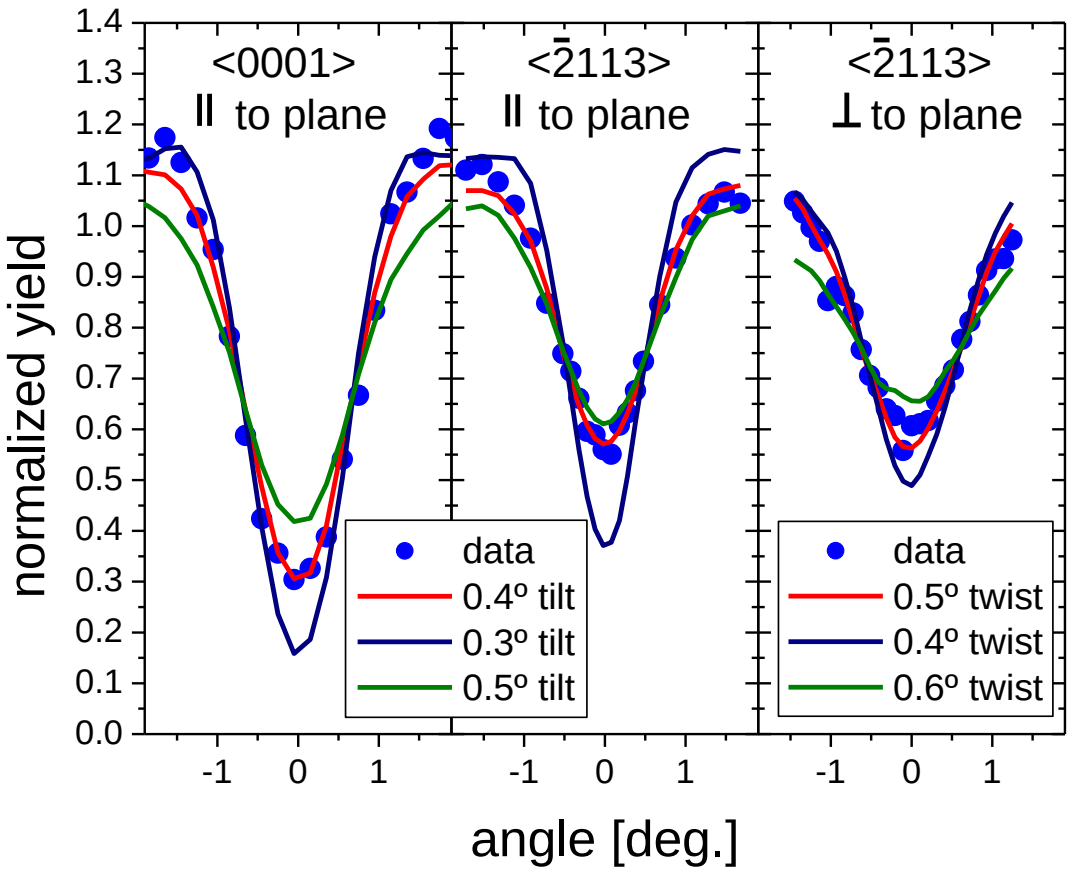
Ga/N

- Preferential orientation of nanowires:

[111] Si || [0001] GaN

[11-2] Si || [10-10] GaN

Mosaicity of Nanowires

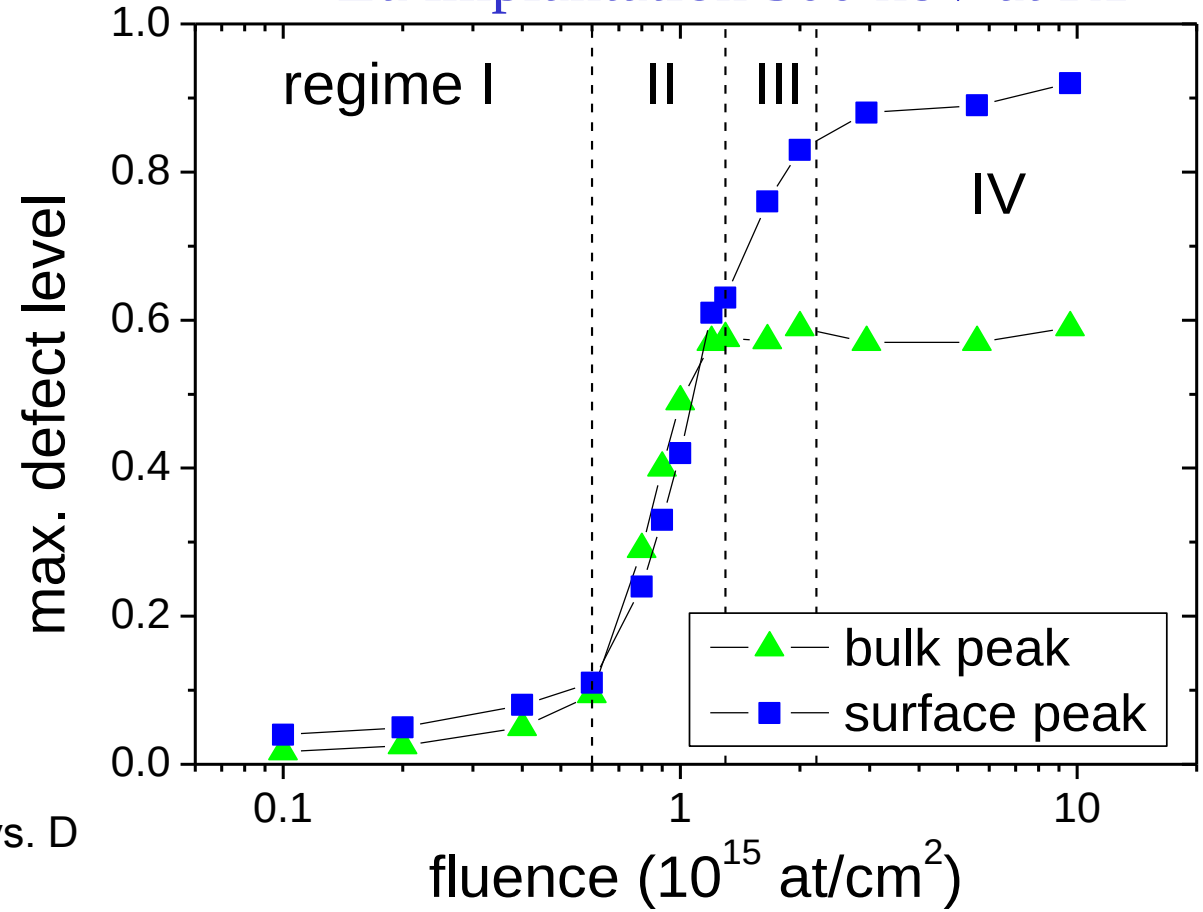


Ion channelling in NWs allows determination of orientation, tilt and twist via Monte Carlo simulations:

- Tilt: 0.4º
- Twist: 0.5º

Implantation damage in GaN

Eu implantation 300 keV at RT



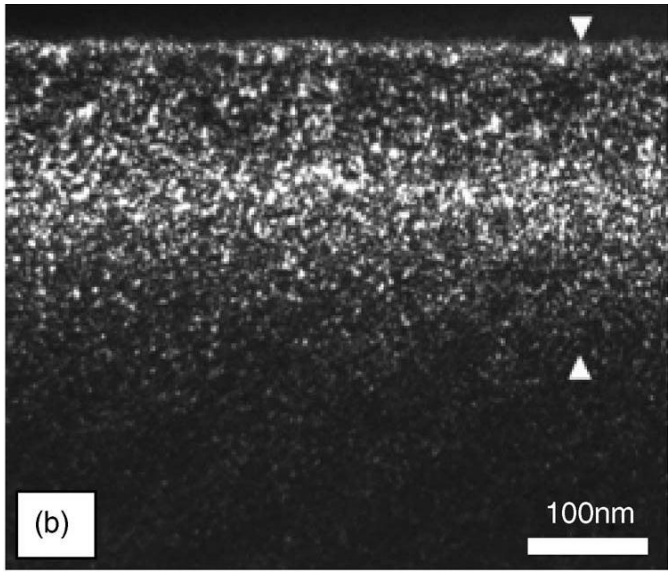
Lorenz et al. J. Phys. D 42 (2009) 165103

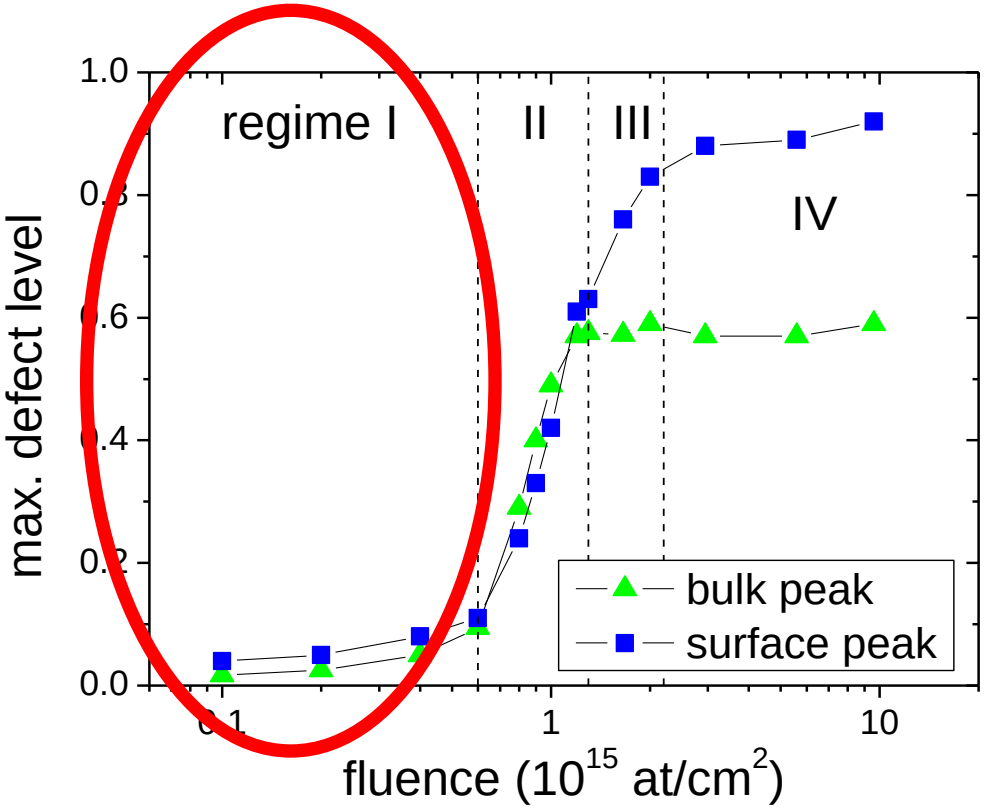
⇒ Sigmoidal shaped damage build-up curve

⇒ Efficient dynamic annealing

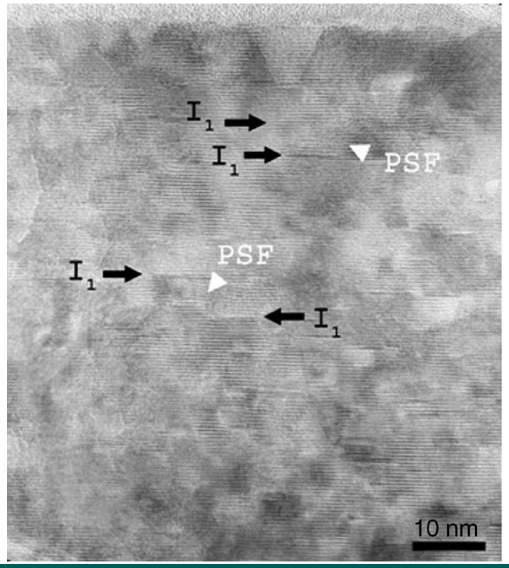
Implantation damage in GaN

TEM
0002
dark field





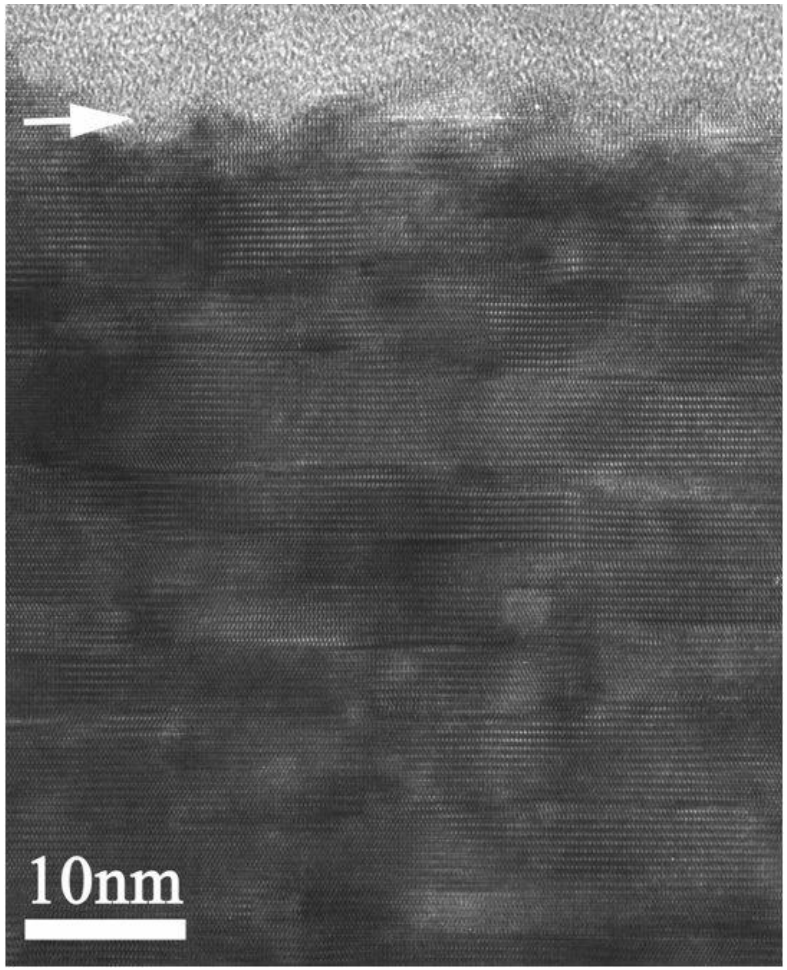
HRTEM

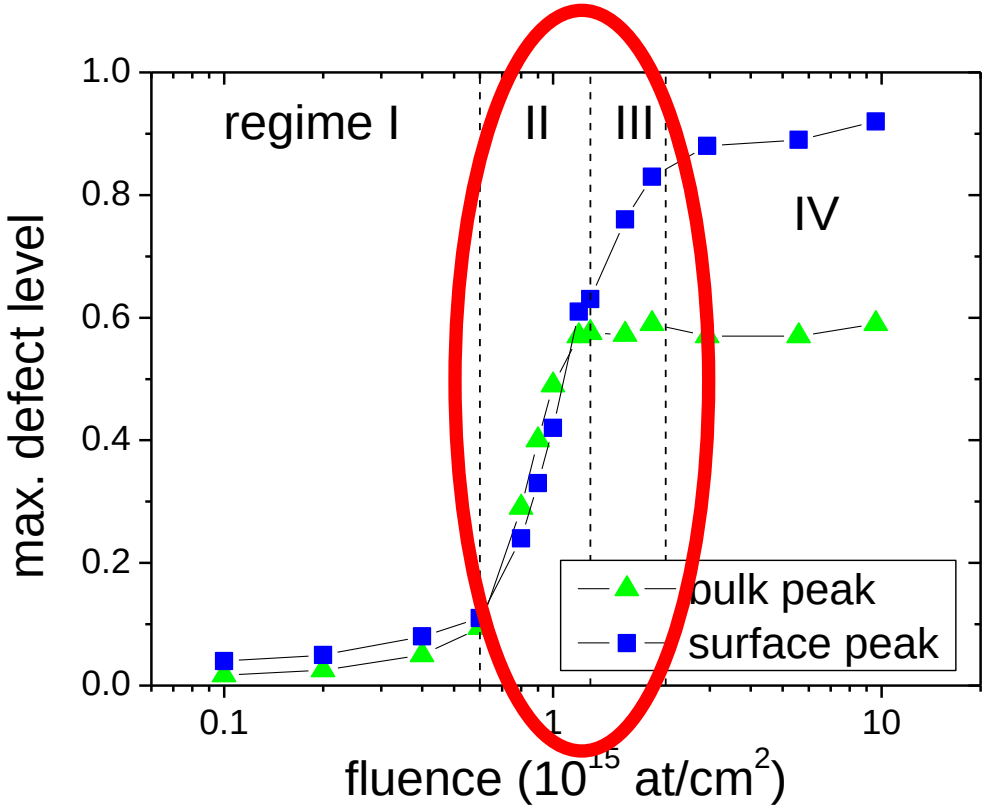


- Point defect clusters
- Low concentration of stacking faults

Implantation damage in GaN

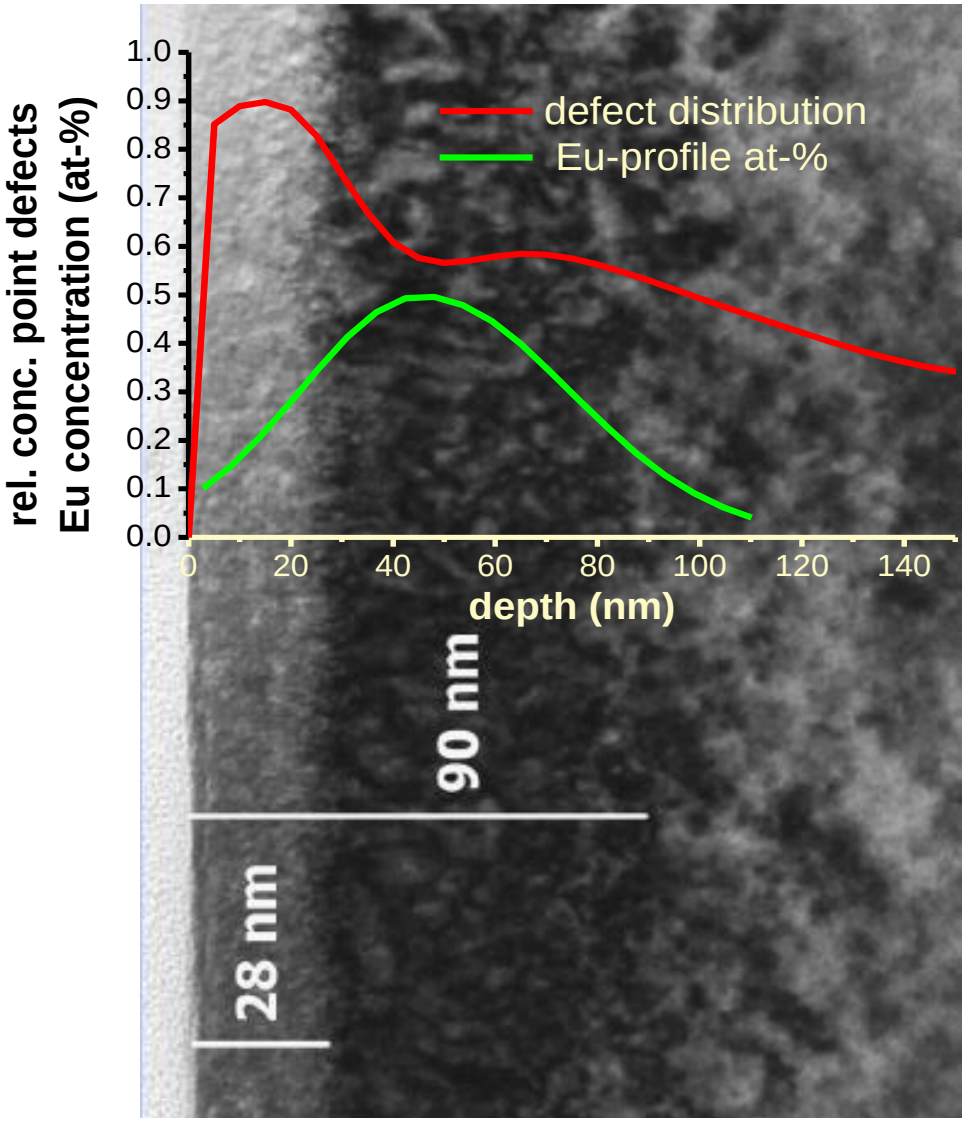
HRTEM

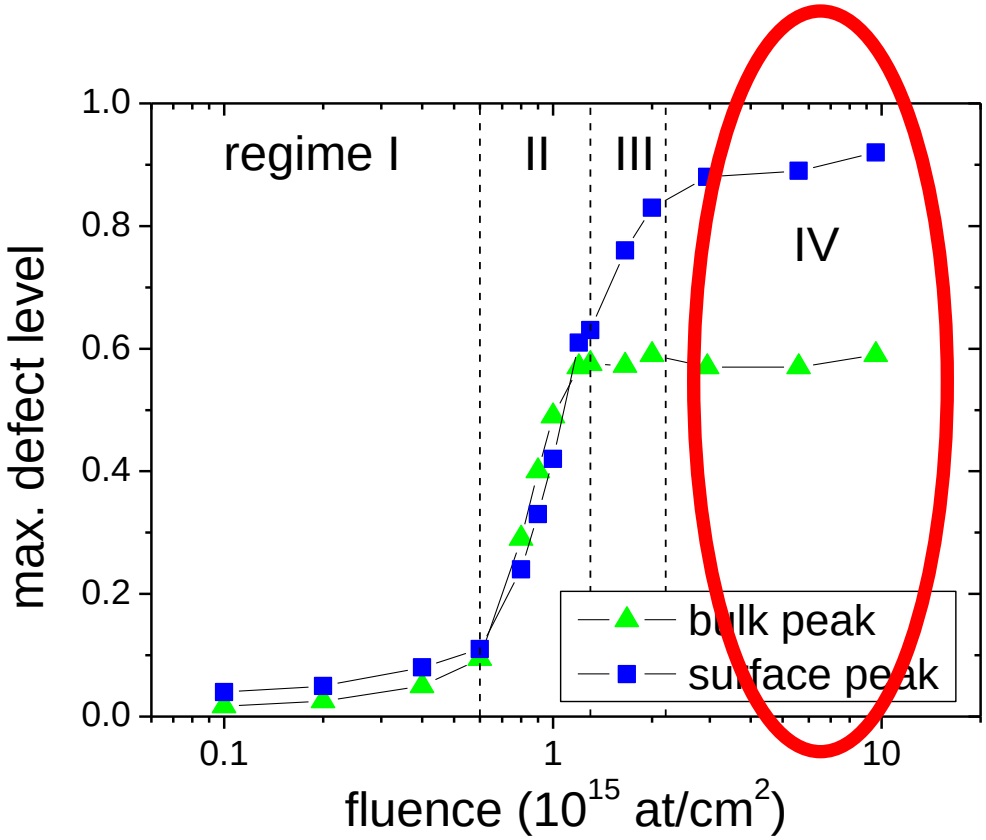




- Increasing number of stacking faults

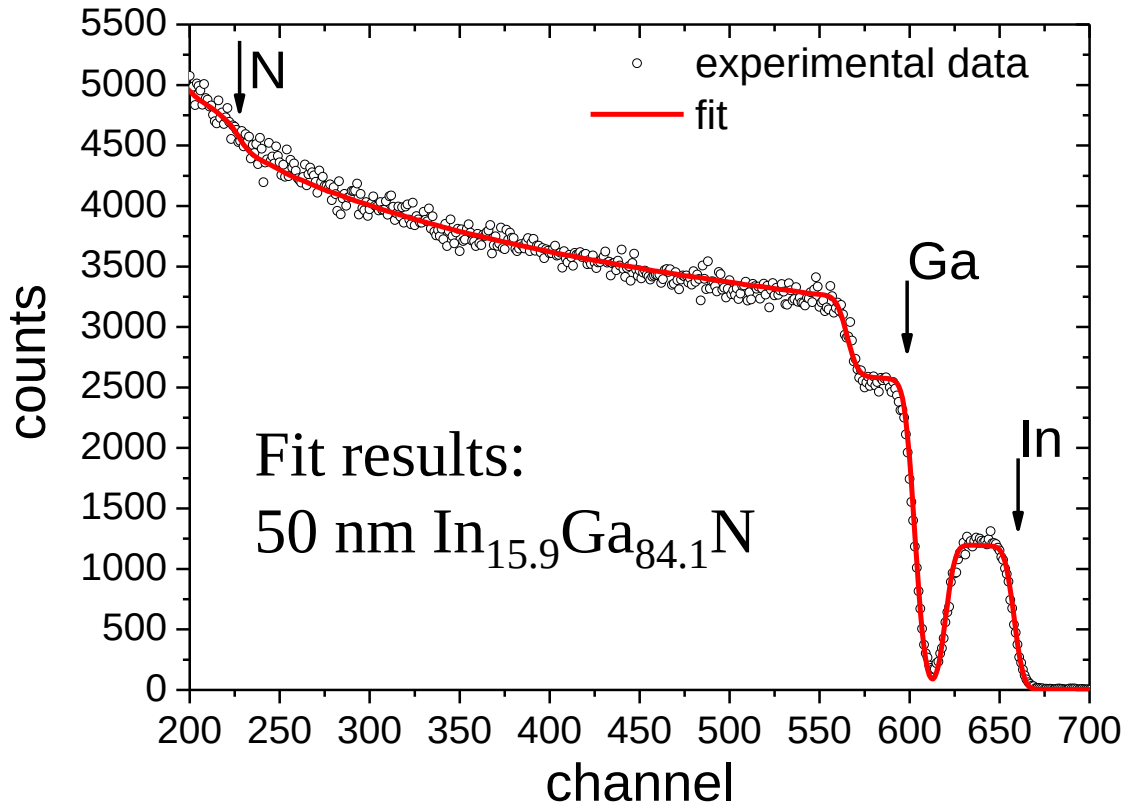
Implantation damage in GaN

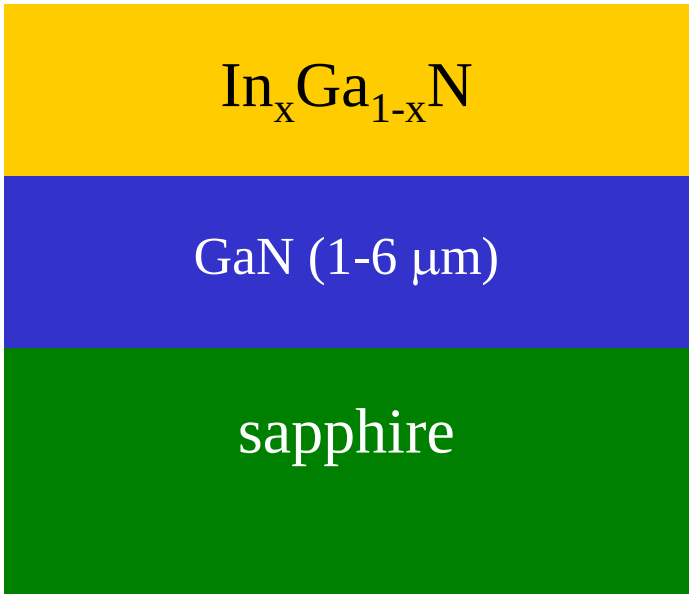




- Nanocrystalline surface layer with voids
- Stacking fault density in bulk saturates

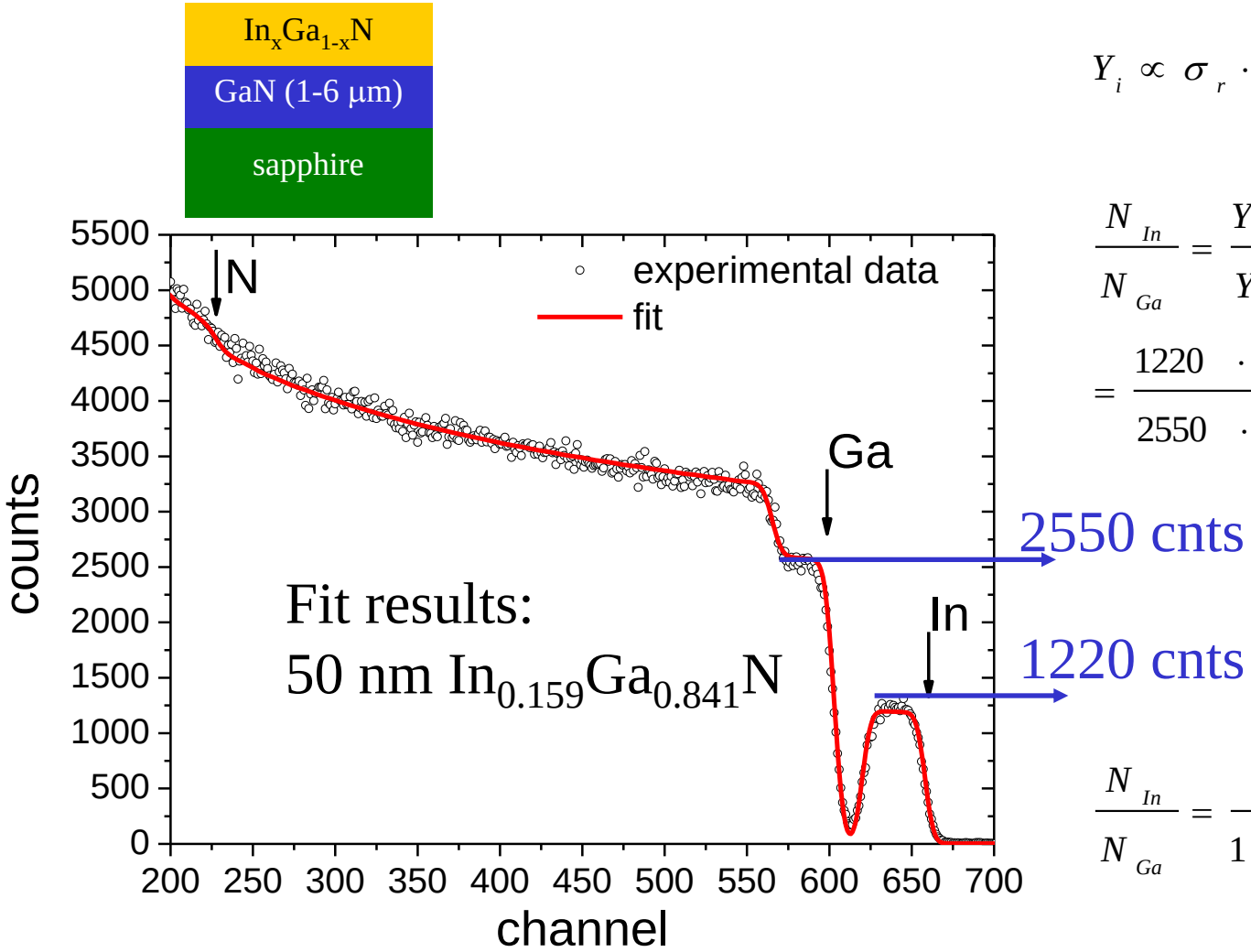
$In_xGa_{1-x}N/GaN$: Thin film





⇒ 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.

$In_xGa_{1-x}N/GaN$: Manual Analysis



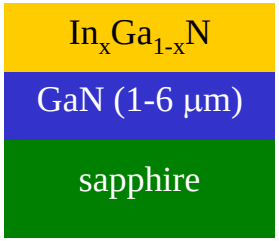
$$Y_i \propto \sigma_r \cdot N_i \qquad [N_i] = \frac{at}{cm^2}$$

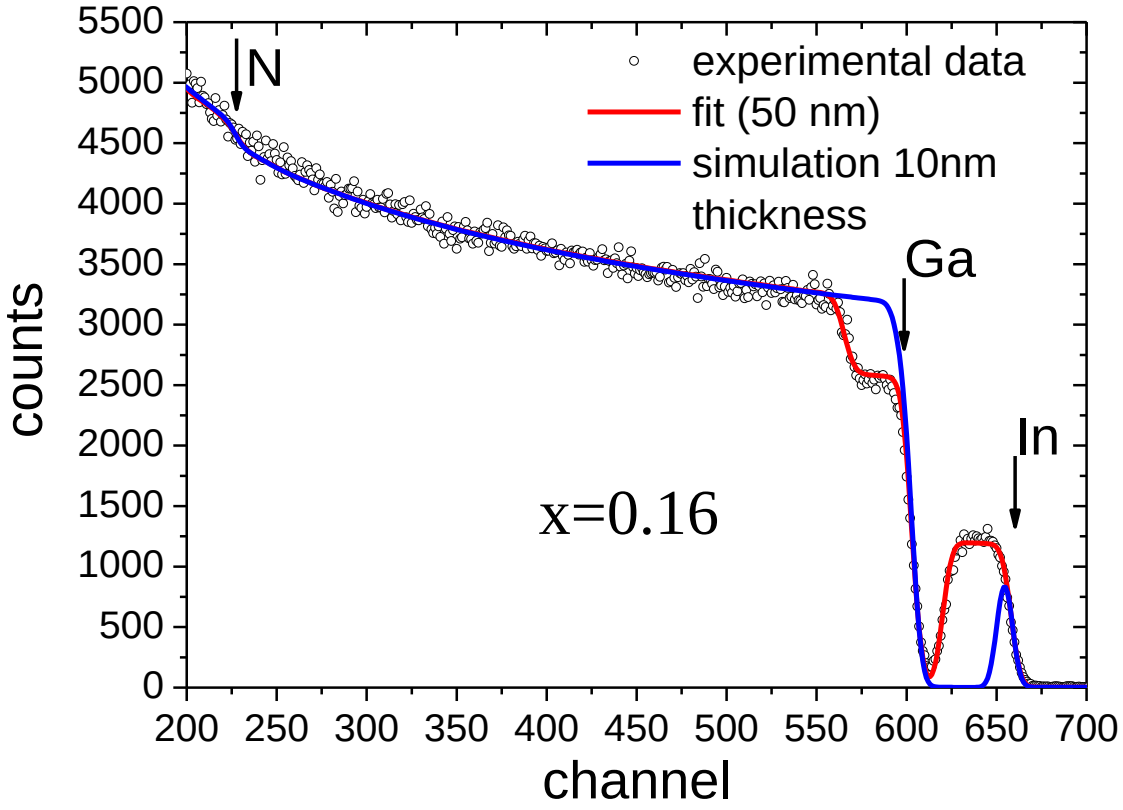
$$\frac{N_{In}}{N_{Ga}} = \frac{Y_{In} \cdot \sigma_r(Ga)}{Y_{Ga} \cdot \sigma_r(In)} = \frac{1220 \cdot 2.482264 \; barn/str}{2550 \cdot 6.221996 \; barn/str} = 0.191$$

$$\frac{N_{In}}{N_{Ga}} = \frac{x}{1-x} \Leftrightarrow x = \frac{\frac{N_{In}}{N_{Ga}}}{(1 + \frac{N_{In}}{N_{Ga}})} = 0.16$$

$\Rightarrow$ Composition from fit and manual analysis match perfectly

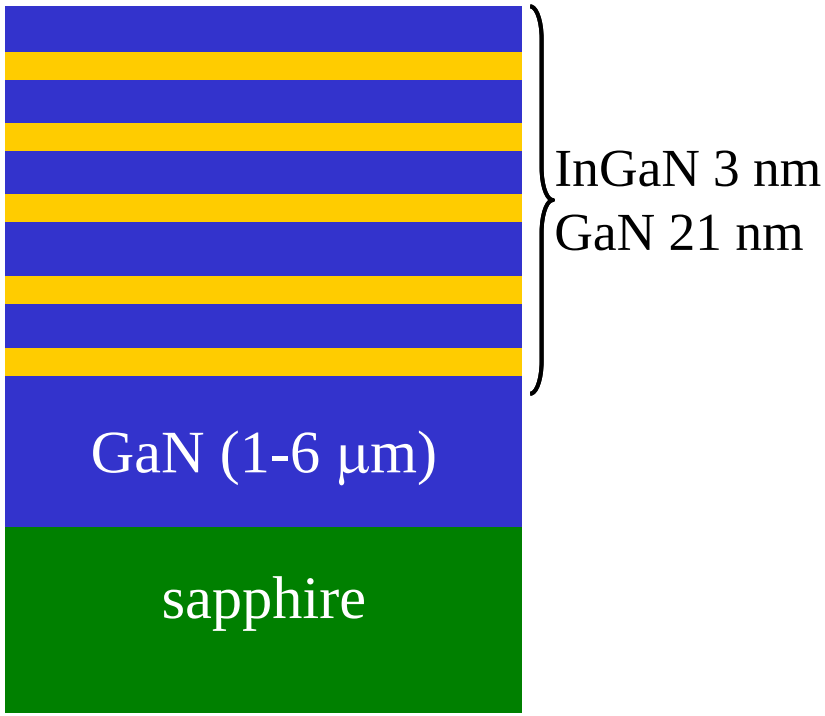
$In_xGa_{1-x}N/GaN$: Going to Nanoscale





⇒ 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.

$In_xGa_{1-x}N/GaN$: Multi Quantum Well (MQW)



5 samples with different InN content

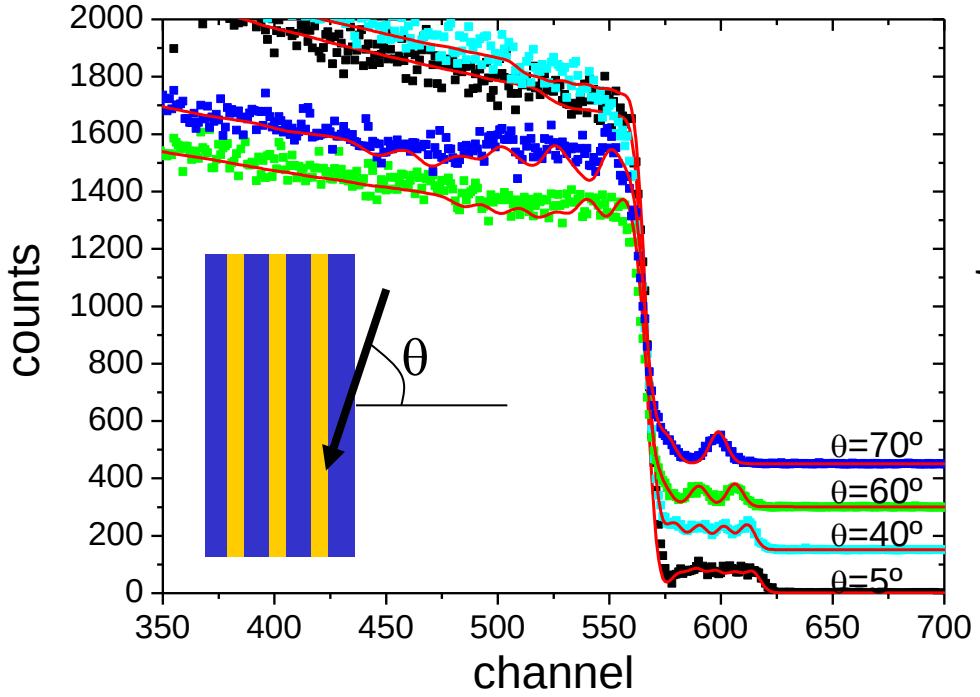
$In_xGa_{1-x}N/GaN$ MQW
5 periods
Nominal QW thickness 3nm
Grown by Metal Organic Chemical Vapour Deposition (MOCVD)

⇒ QW thickness and QW composition difficult to measure with most techniques

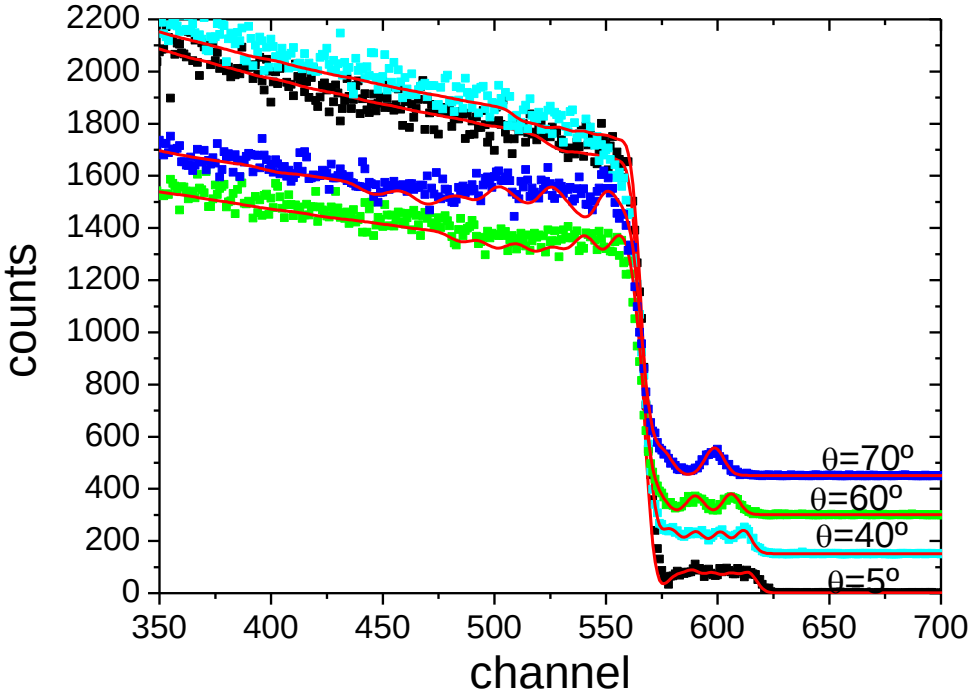
- XRD measured the period and average composition
- PIXE, WDX measures the total In-content; QW thickness needs to be known
- SIMS suffers from artefacts due to contaminations from the sides
- TEM+EDX possible but very time consuming

$In_xGa_{1-x}N/GaN$: Multi Quantum Well (MQW)

Fit using ~3nm QW, x=0.11



Fit using ~5nm QW, x=0.07

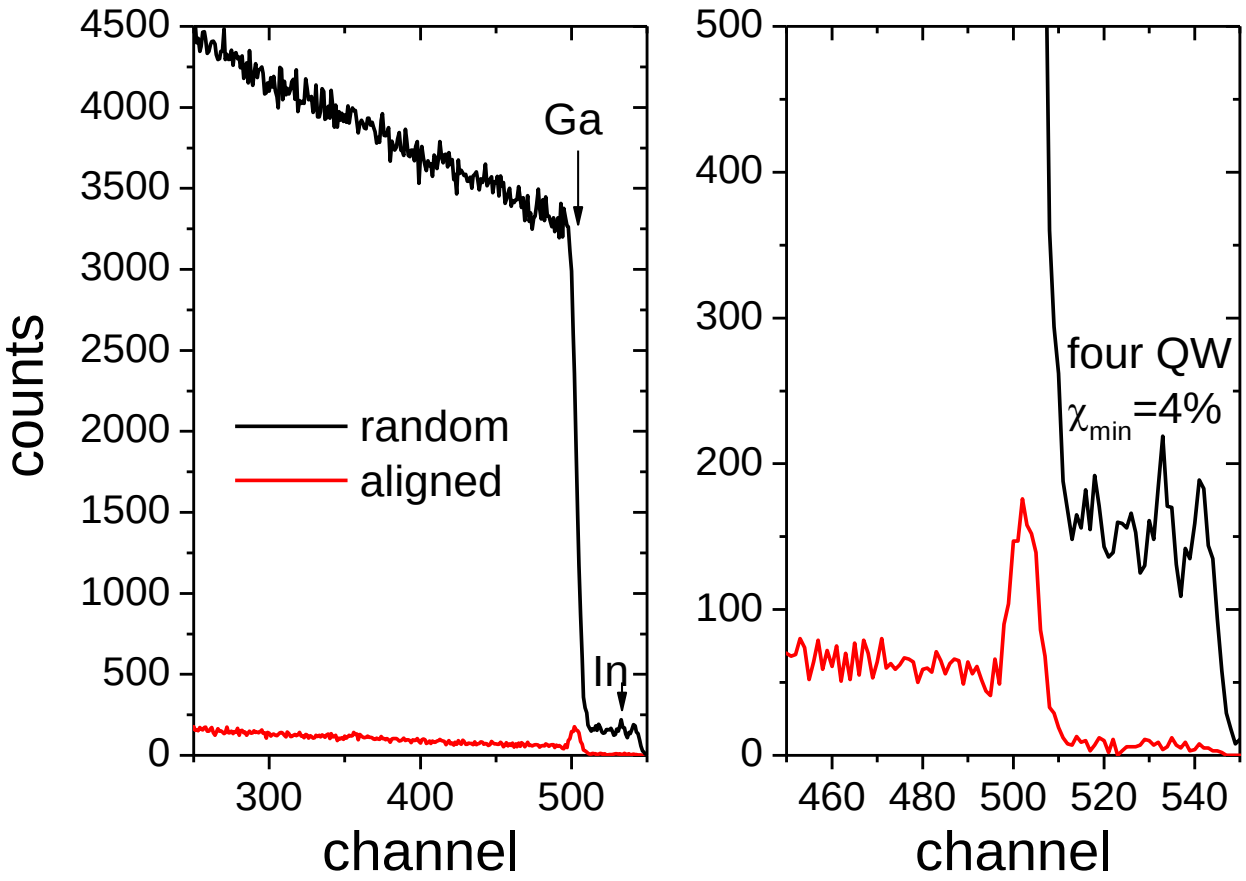


⇒ Composition and thickness cannot be determined unambiguously (complementary measurements necessary e.g. TEM).

⇒ Period, total InN content and "product" thickness × composition.

⇒ Assuming the nominal thickness of 3 nm, x was determined to vary from 2 to 14 %

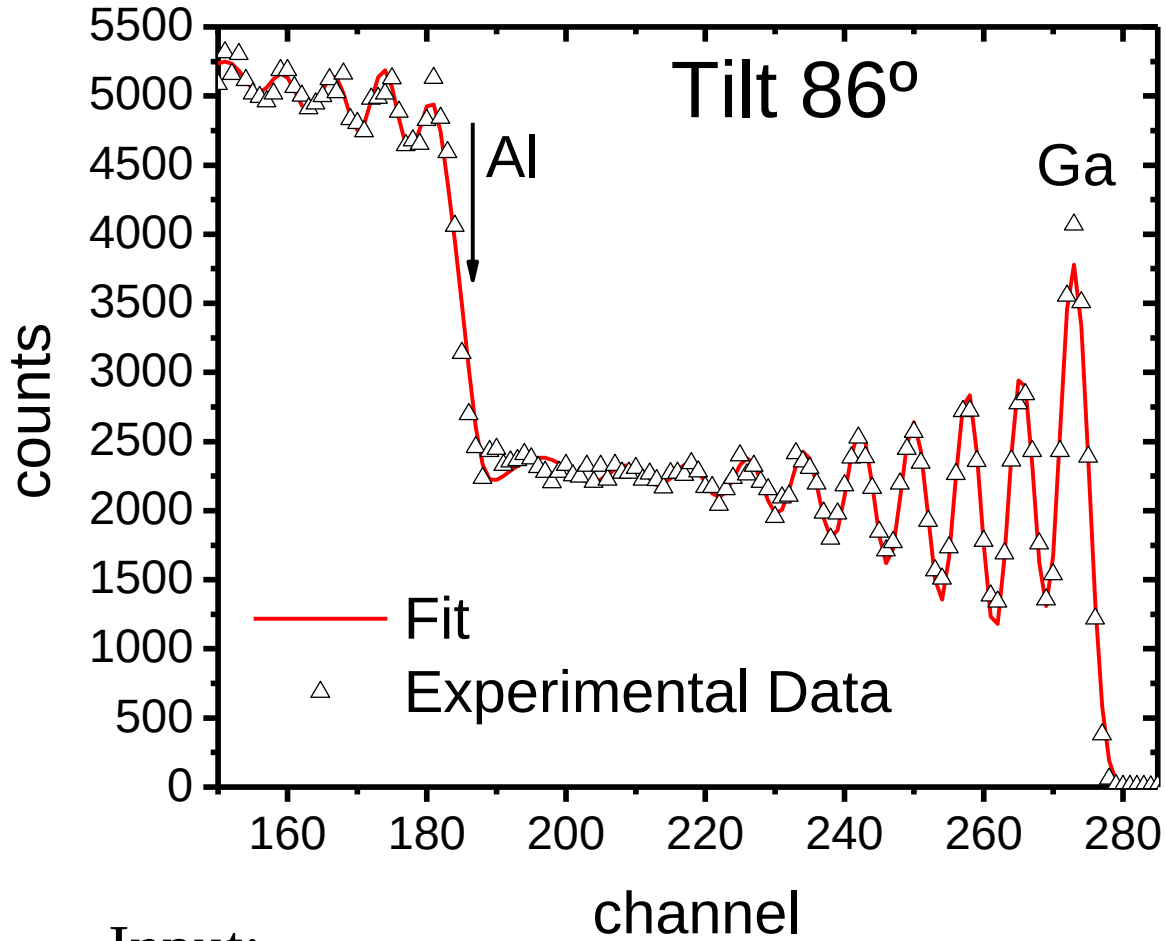
Crystal Quality in QWs



⇒ Minimum yield for Ga: < 2% in all samples

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

Grazing Incidence



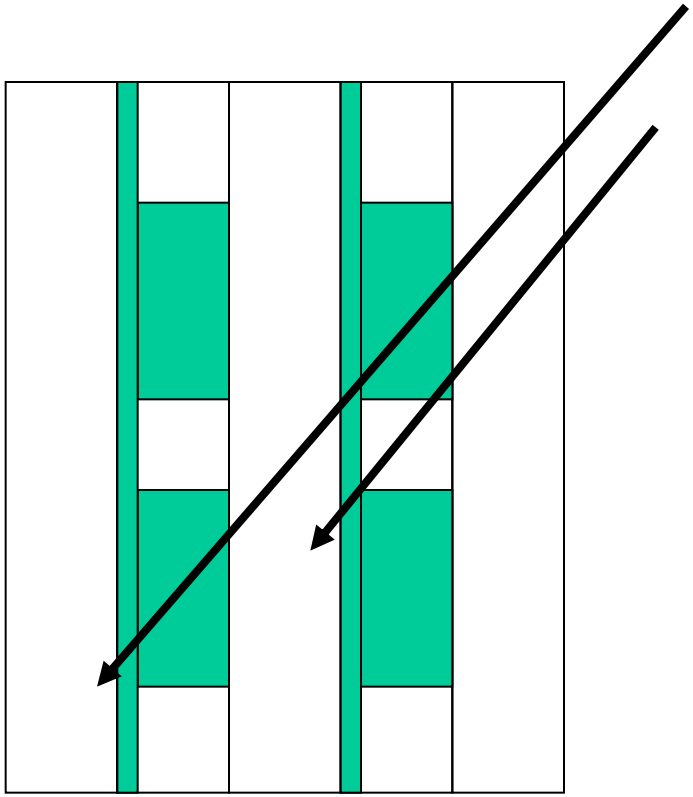
Layer	Material	Thickness [nm]
1	GaN/AlN	3.435
2	AlN	4.558
3	GaN/AlN	2.669
4	AlN	5.202
5	GaN/AlN	2.642
6	AlN	5.082
7	GaN/AlN	2.557
8	AlN	5.037
9	GaN/AlN	2.663

Input:
Cylindrical QD: Height 2.6 nm
Radius 8.5 nm

$\Rightarrow$ 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

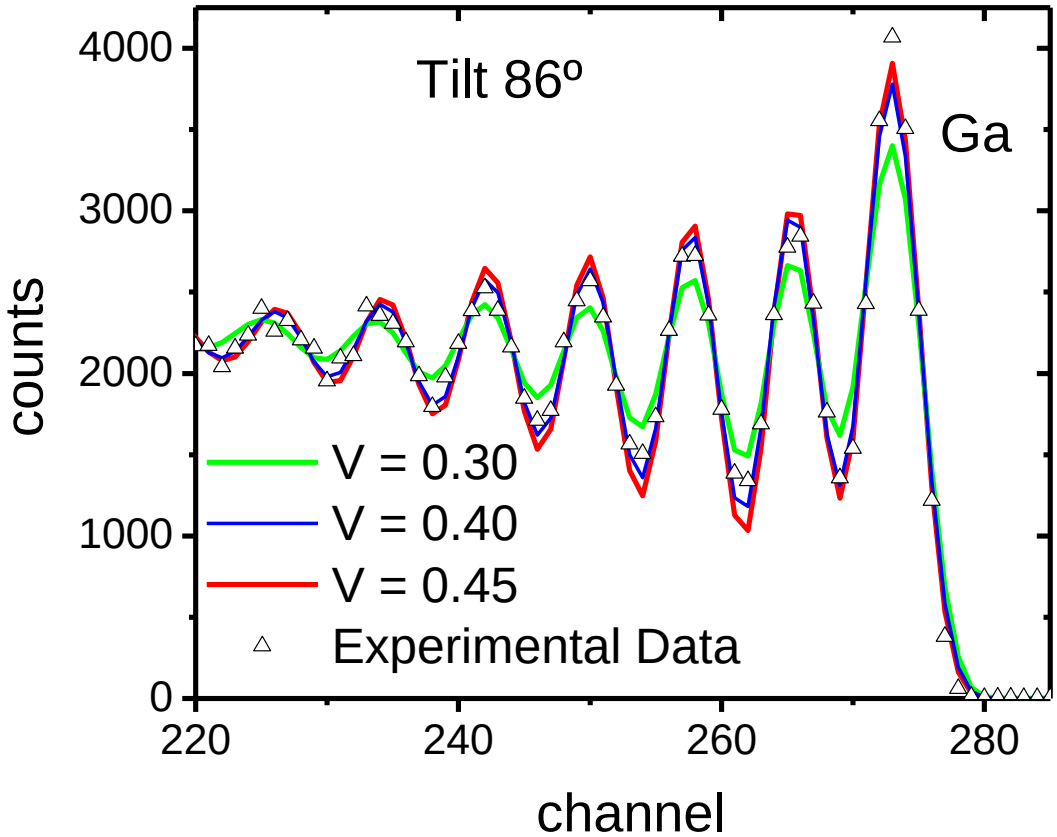


NDF calculates:
- Quantity of material crossed
- Energy spread due to difference in stopping power

→ volume fraction

[1]N. Barradas et al. APL 71 (1997) 291.
[2]J.P. Stoquert et al. Phys. Rev. B 66 (2002) 144108.
[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)