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XRD Investigation of crystal defects in semipolar and nonpolar GaN

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Nonpolar & semipolar III-Nitrides

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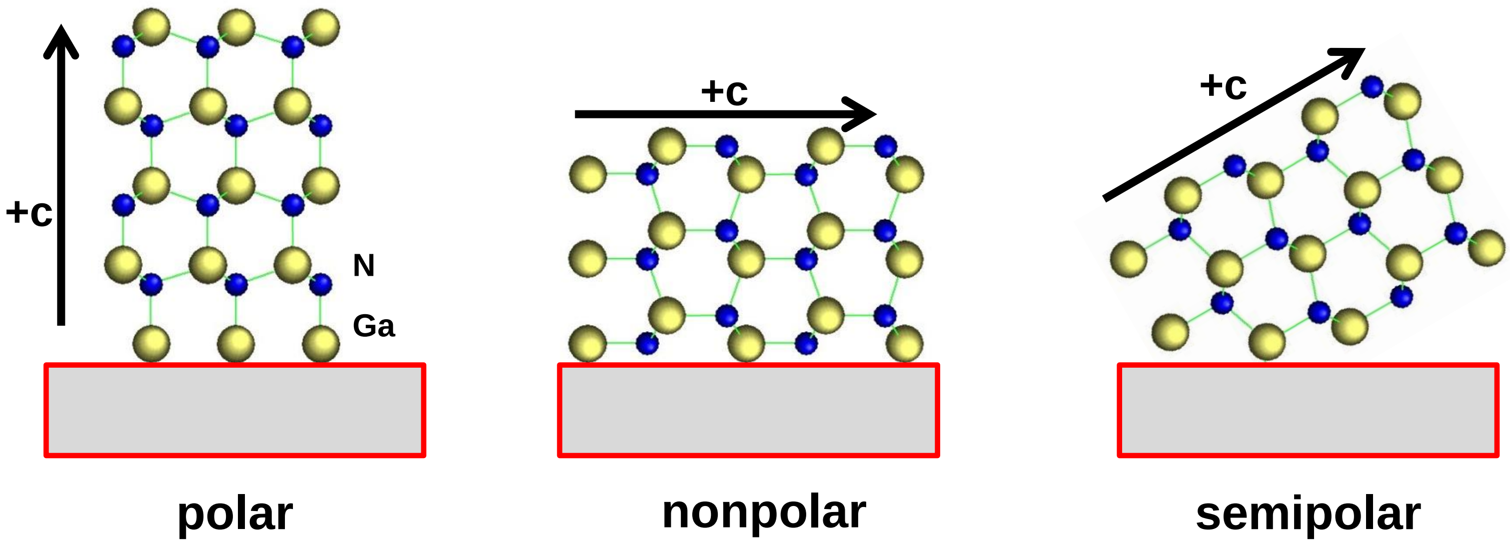
III-N = wurtzite: polar structure → Polarization along the c-axis



Growth along nonpolar and semipolar orientations:

→ Internal polarization in growth direction reduced

→ Reduced Quantum Confined Stark Effect (QCSE)!

Defects in non c-plane GaN

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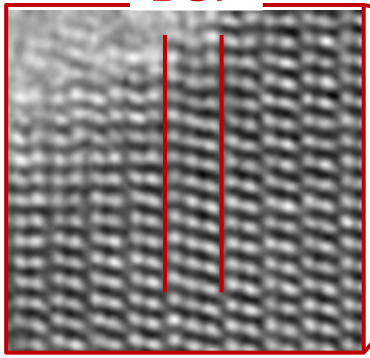
Heteroepitaxy

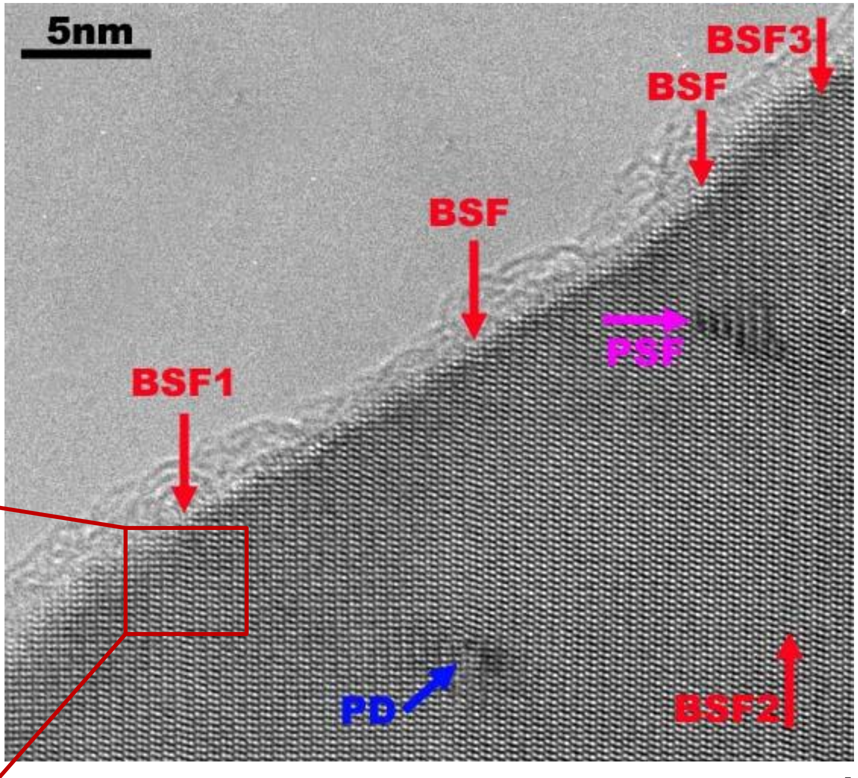
- Difference in structure, lattice parameters, chemistry, … with GaN

→ High density of structural defects

- Basal plane stacking faults (**BSF**)
- Prismatic planes stacking faults (**PSF**)
- Partial dislocations (**PD**)

e.g. nonpolar a-GaN on r-Sapphire





Plan view HRTEM image, [11-20] zone axis[1]

[1] P. Vennéguès et al., **P**hys. Stat.sol. C **3/6**, 1658-1661 (2006).

Defects in non c-plane GaN

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Heteroepitaxy

- Difference in structure, lattice parameters, chemistry, … with GaN

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- Basal plane stacking faults (**BSF**)
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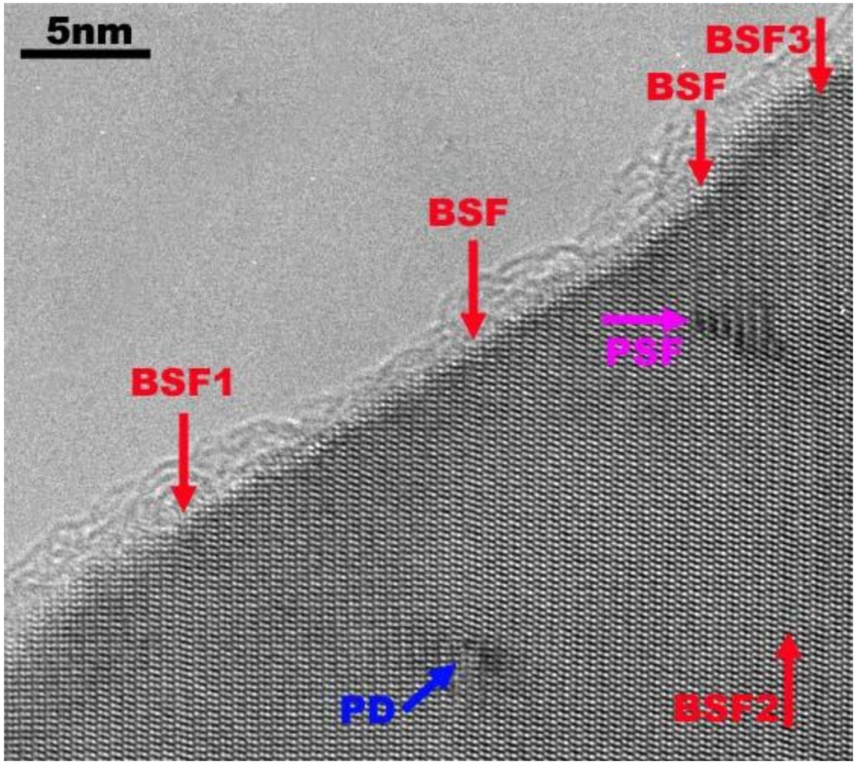
Defects…

- Cause local strain
- Act as non-radiative centres

→ Negative impact on LED performance

→ Reduction of defects necessary

e.g. nonpolar a-GaN on r-Sapphire



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Sample overview

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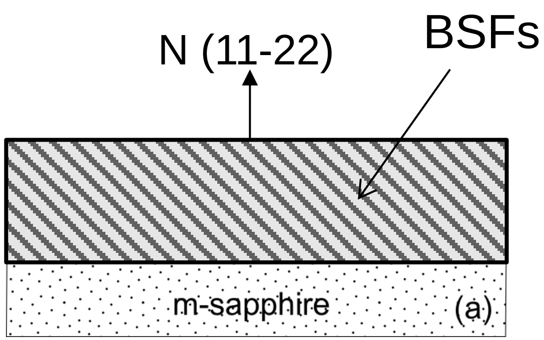
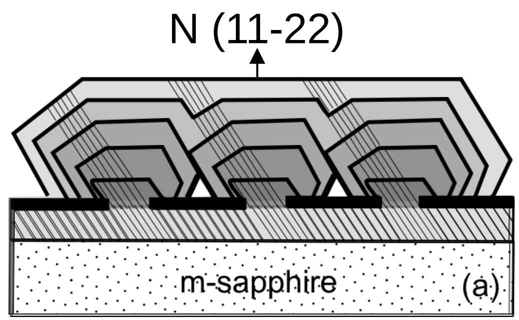
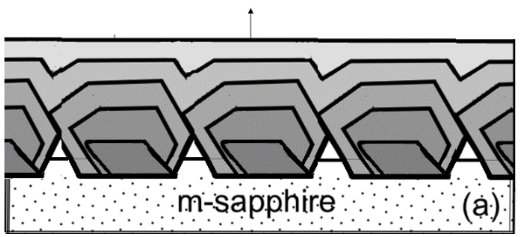


Normal overgrowth



AlN & SiN_x interlayer



Patterned substrates

BSF: (11-22) GaN on m-Sapphire by TEM

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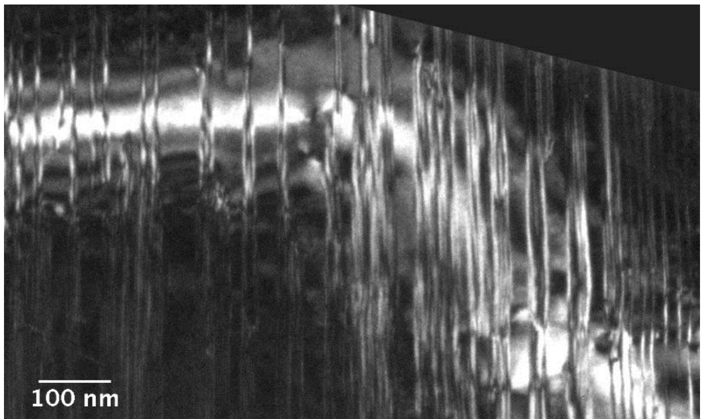
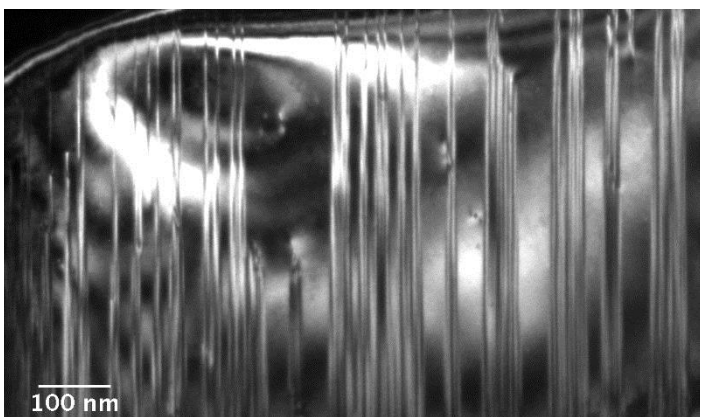
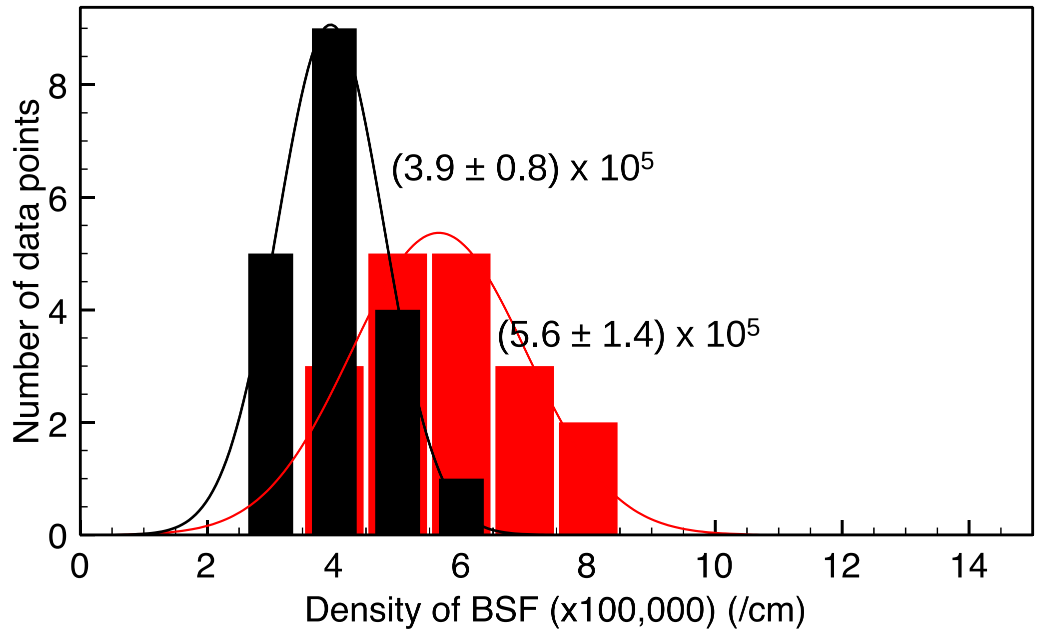


No interlayers



3 x low temp. AlN + 3 x SiN_x interlayer



Plane view TEM:

- Interlayer reduce BSF by 30%

→ TEM gives good results, but with long feedback times

→ Need of a faster method

BSF: a-GaN analysis by XRD

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X-ray diffraction:

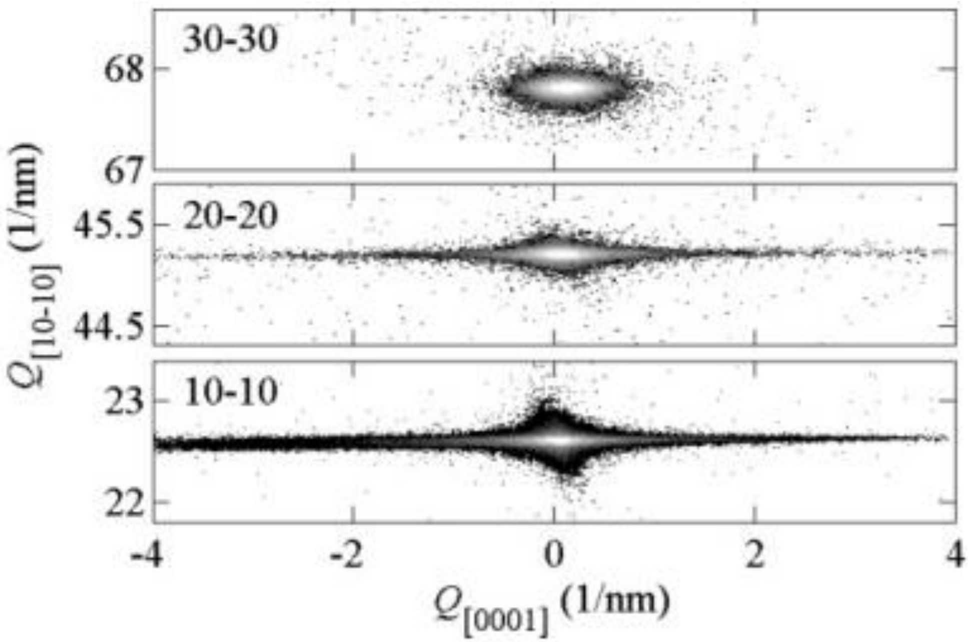
- Non-destructive
- Fast
- BSFs cause streaking of selected X-ray reflections parallel to c-axis,

- if **b**·**g** ≠ integer

→ if **g** ≠ m·{11-20} + n·{0002}
+ o·{30-30}

→ Can be used to estimate BSF densities

Parallel to c-axis



Barchuk et al., Physical Review B 84 (2011), 094113

Modified Williamson-Hall Plot

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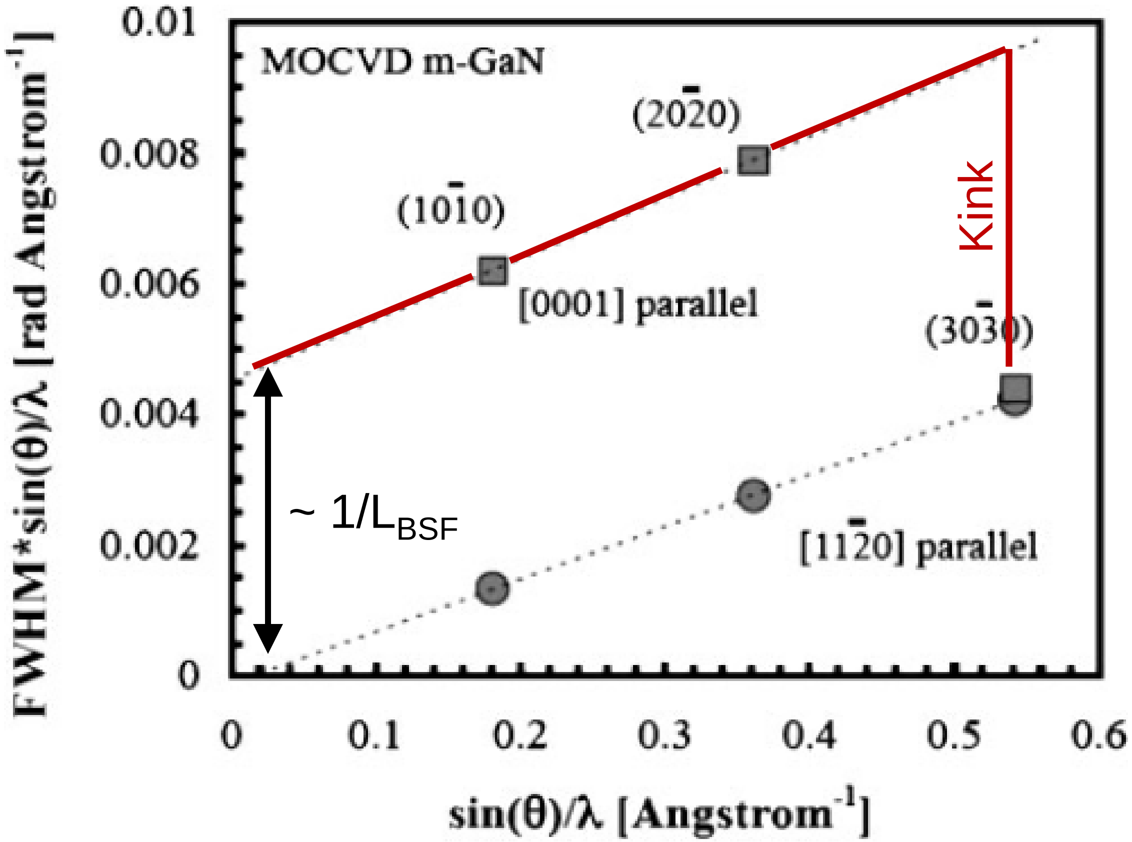
Method well known for non-polar orientations



- Measuring higher order Bragg reflections (h0-h0), h = 1, 2, 3
- BSF density:
  - Kink: > 10^4 cm^{-1}
  - No kink < 10^4 cm^{-1}

[1] McLaurin et al., Jpn. J. Appl. Phys. **47**, 5429 (2008).

Modified Williamson-Hall Plot

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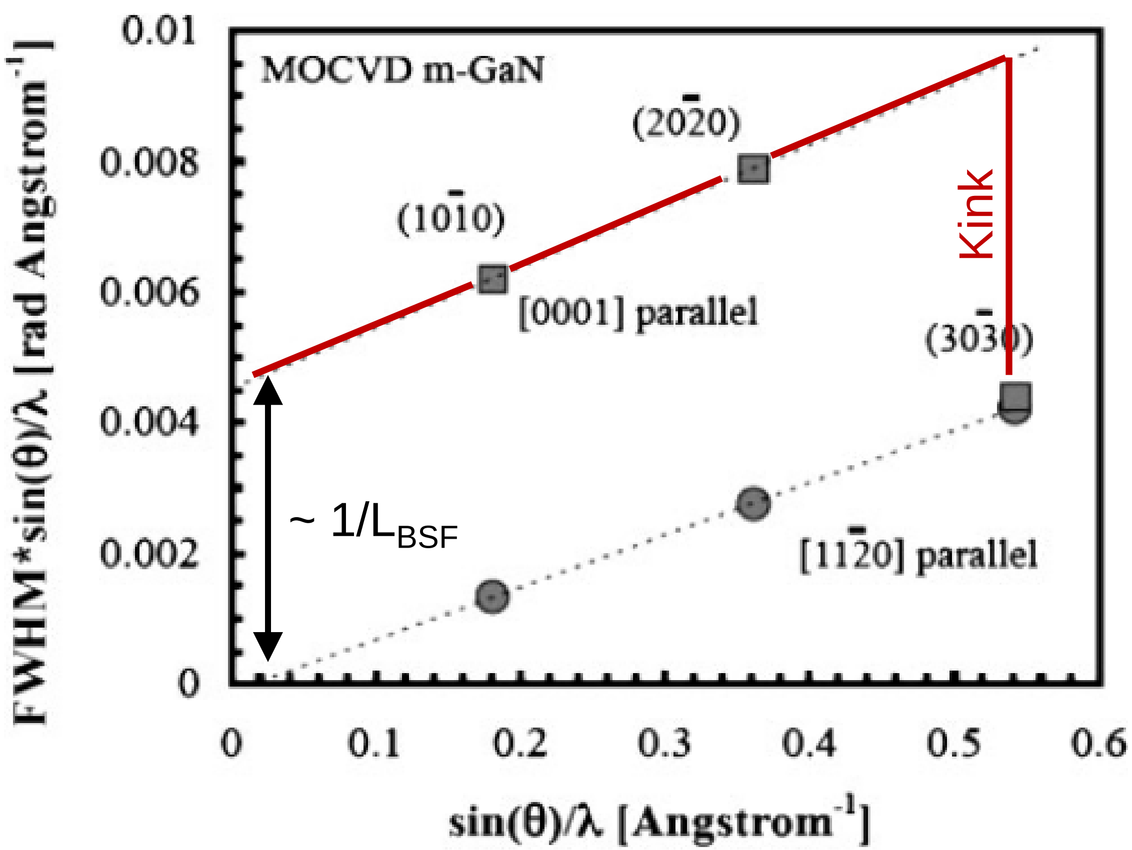

- Measuring higher order Bragg reflections (h0-h0), h = 1, 2, 3
- BSF density:
  - Kink: > 10^4 cm^{-1}
  - No kink < 10^4 cm^{-1}
- Semipolar GaN:
  - Measurement of higher order reflection and/or parallel to c-axis often not possible
  - Influences by other defects

[1] McLaurin et al., Jpn. J. Appl. Phys. **47**, 5429 (2008).

BSF analysis for semipolar GaN

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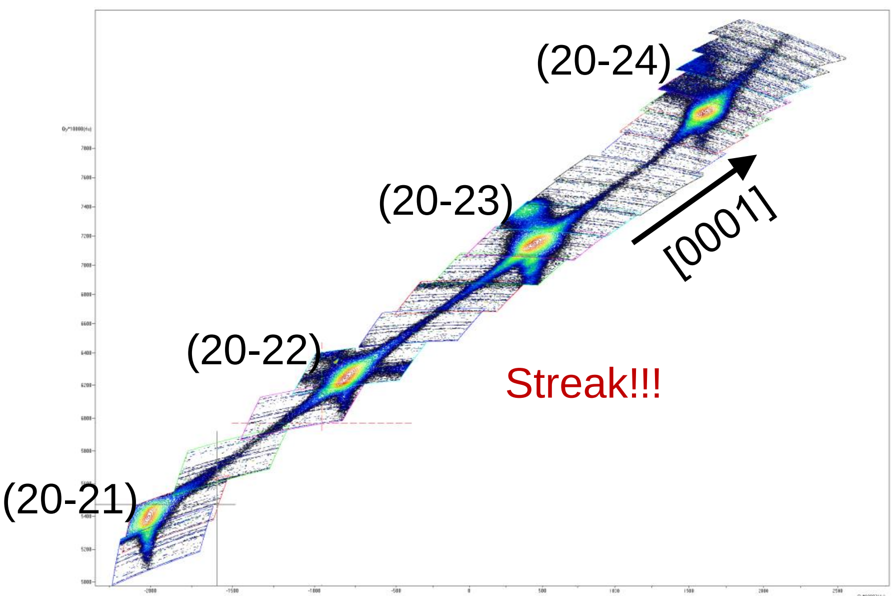
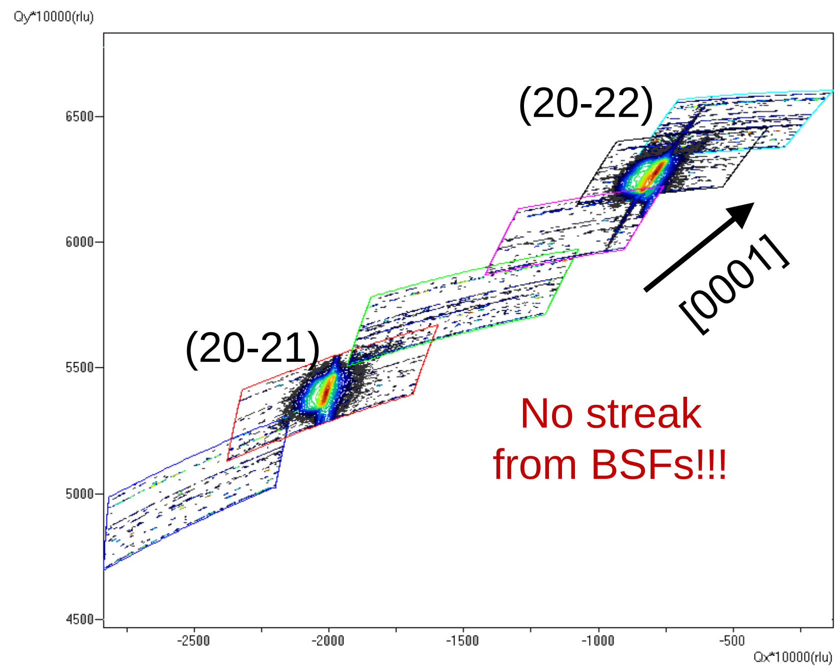
- Measuring different reflections along the streak, e.g. (20-2L), L = 1, 2, 3, …

GaN/sapphire
with very high BSF density ($10^5 cm^{-1}$)



GaN on pattern template
with low BSF density ($580 cm^{-1}$)



Compare of streak profiles

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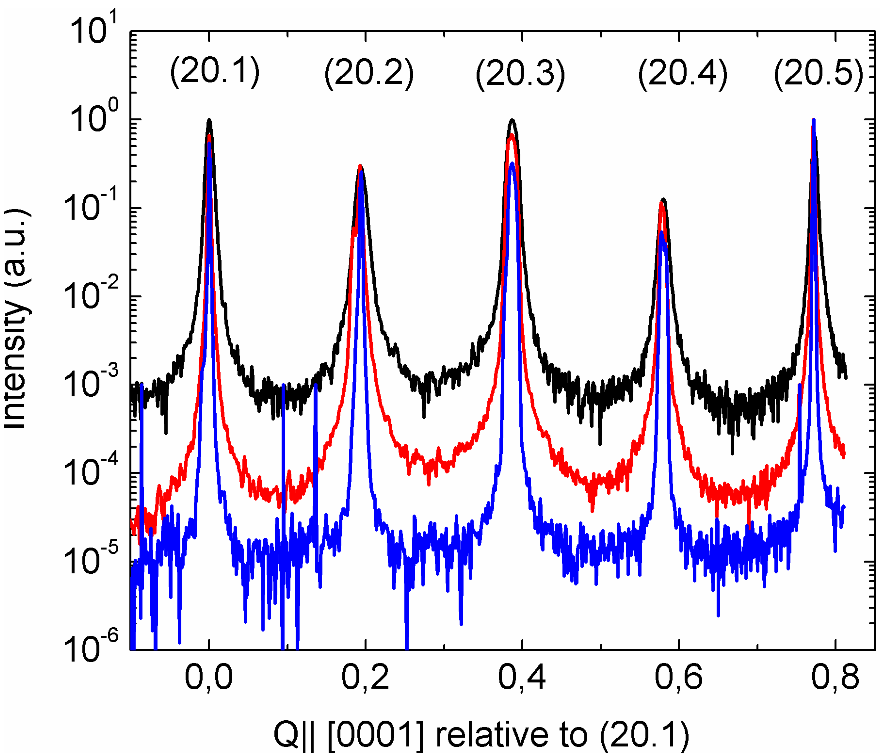

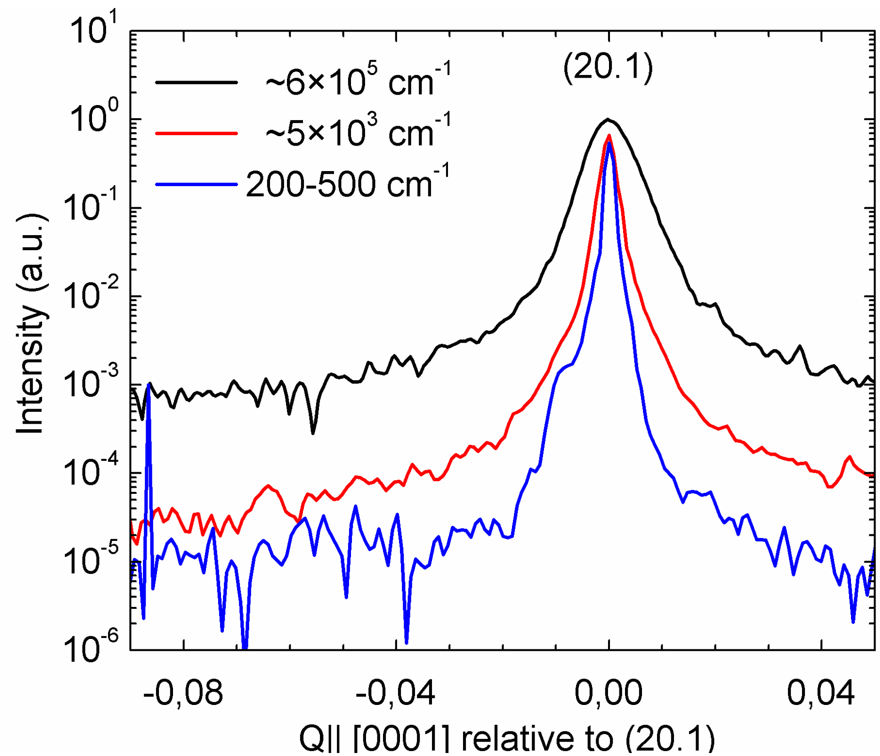

- Characteristic broadening found between the peaks

→ Now a model needs to be applied

Kinematic theory of diffraction[1]

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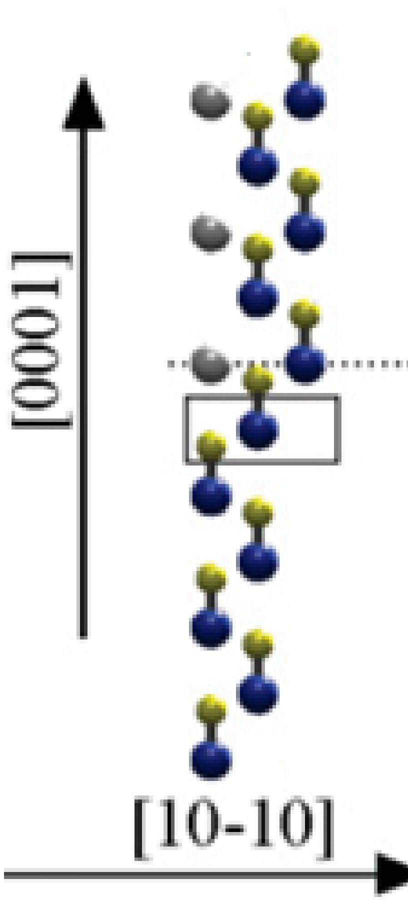
I_1 type   Seq.



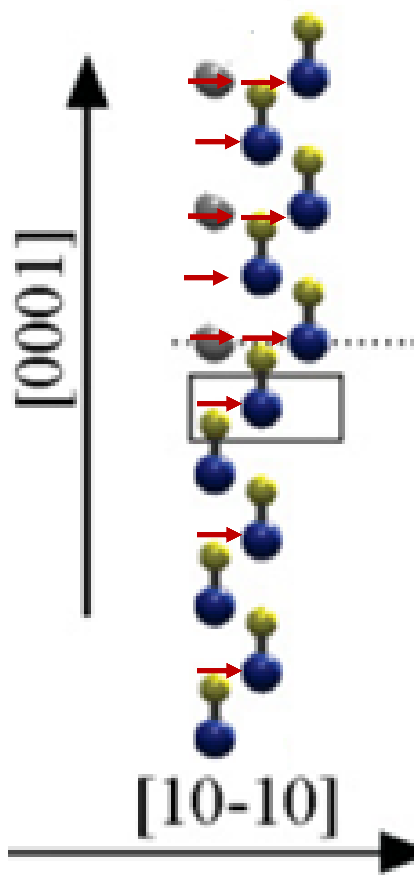
C
B
C
B
C
B
A
B
A
B
A

- BSF = stacking error in a sequence of Ga-N-bilayers

[1] Barchuk et al., Physical Review B **84** , 094113 (2011).

Kinematic theory of diffraction[1]

I_1 type



Seq.	$\sigma \times \mathbf{p}$
C	2
B	1
C	2
B	1
C	2
B	1
A	0
B	1
A	0
B	1
A	0

- BSF = stacking error in a sequence of Ga-N-bilayers
- Displacement given by vector $\sigma \times \vec{\mathbf{p}}$

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Kinematic theory of diffraction[1]

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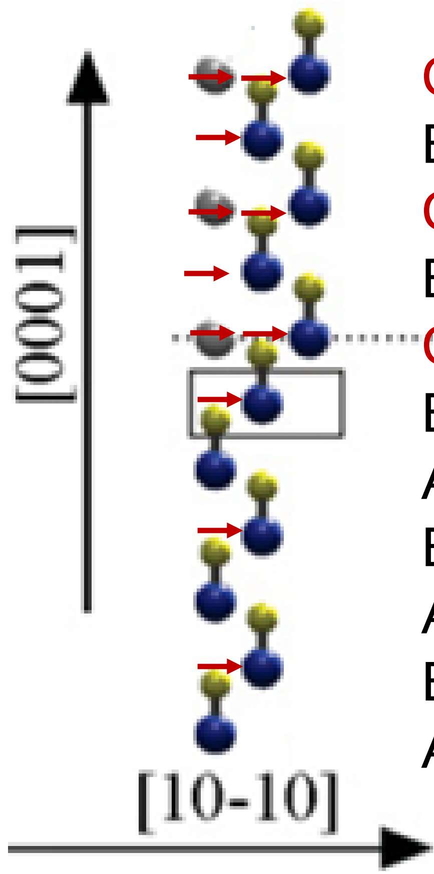

I_1 type	Seq.	$\sigma \times \vec{\mathbf{p}}$
	C	2
	B	1
	C	2
	B	1
	C	2
	B	1
	A	0
	B	1
	A	0
	B	1
	A	0

- BSF = stacking error in a sequence of Ga-N-bilayers
- Displacement given by vector $\sigma \times \vec{\mathbf{p}}$
- Assuming random distribution of BSFs in a long sequence (e.g. 10^3 bilayers)

$$Int. \propto E(Q)^2 \propto \left(\sum \exp(-iQ \cdot \sigma p) \right)^2$$

- Diffuse scattering from stacking faults along c-direction

[1] Barchuk et al., Physical Review B **84** , 094113 (2011).

Theory from Barchuk et al.

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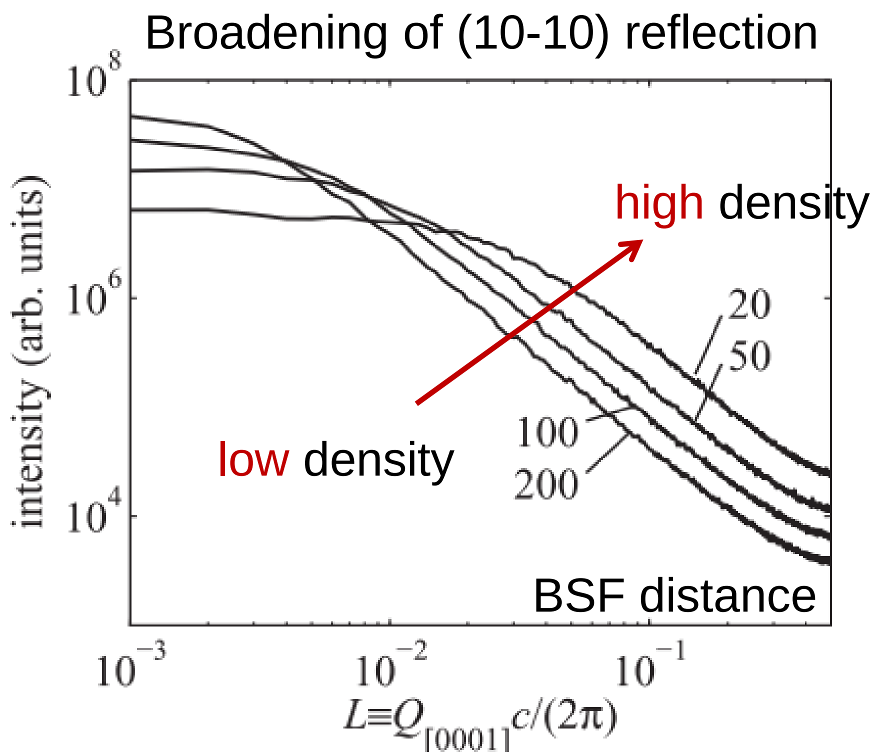

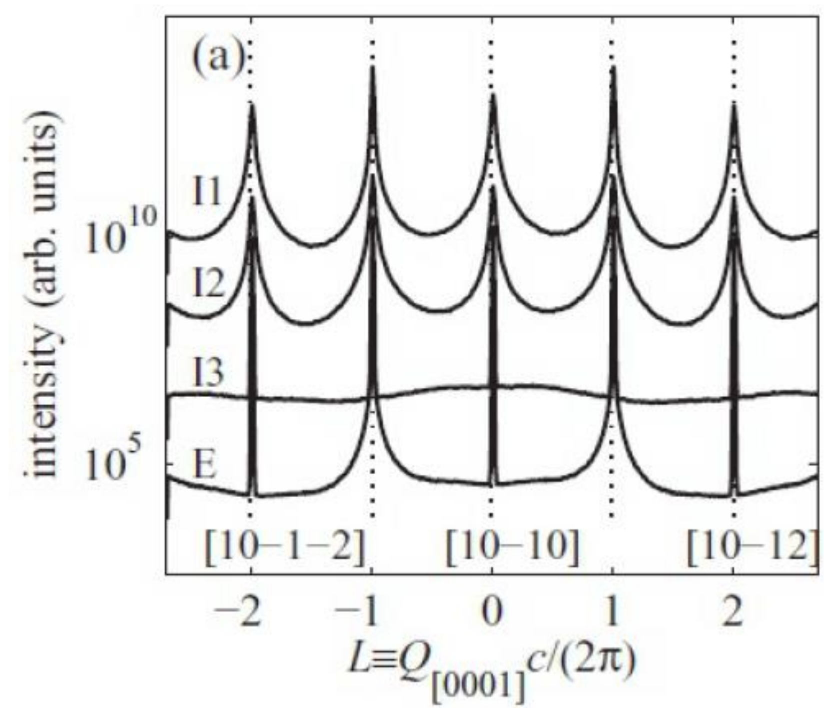

- High density → larger FWHM
- Different BSF types → different peak shapes
- BSF density and type from shape of BSF-streak

[1] Barchuk et al., Physical Review B **84** , 094113 (2011).

Summary

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- Defect structure of several semipolar and nonpolar samples were analysed
- TEM shows reduced BSF density for semipolar GaN templates
  with AlN & SiN_X interlayers
- BSFs cause streaking of selected X-ray reflections parallel to c-axis
- Streaking can be described by kinetic scattering theory
  & can be used to estimate BSF type and density

Future work

- Simulation of streaking based on kinetic X-ray scattering theory
- Investigation of the influence of other defects on the broadening,
  e.g. prismatic stacking faults