Summer School on the physics and applications of nitrides

Structural characterization I X-ray diffraction

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Introduction

- W. Röntgen discovered X-rays in 1895.
- 1912: first X-ray diffraction by crystals (proved the wave nature of X-rays).
- Widely used to image the inside of objects.
- A powerful tool to investigate the structure of ordered matter.



Japanese artist Iori Tomita

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Introduction

X-rays wavelength ≈ interatomic distances in crystals

Type of property	General property	Specific property
Macroscopic	Shape	Layer thicknesses
	Composition	Structural phase
	-	Elements present
		Phase extent
	Form	Amorphous
		Polycrystalline
		Single crystal
	Orientation	General preferred texture
		Layer tilt
	Distortion	Layer strain tensor
		Warping
	Homogeneity	Between analysed regions
	Interfaces	Interface spreading
	Density	Porosity
		Coverage



P. F. Fewster, Rep. Prog. Phys. **59** (1996) 1339–1407.

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Structural characterization I: X-ray diffraction

X-ray diffraction a single-crystalline core-shell Ag/Au nanowire (ID01/ESRF, M.-I. Richard). Ction GaNex School 3

Type of property	General property	Specific property
Microscopic	Shape	Average crystallite size
	-	Crystallite size distribution
	Composition	Local chemistry
	Orientation	Crystallite tilt distribution
	Distortion	Crystallite lattice strain
		Crystallite strain distribution
		Dislocation strain fields
		Point defects
		Cracks
		Strain from precipitates
	Interfaces	Roughness
	Homogeneity	Distribution within region of sample studied



I. Basics

II. The diffractometer

III. Diffraction from materials

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1. Crystallography or the direct space

2. Diffraction or the reciprocal space

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Some definitions

Crystal

"A crystal is a region of matter within which the atoms are arranged in a three-dimensional translationally periodic pattern" Buerger (1956).



Lattice

A lattice is "an imaginary pattern of points" in which all points have the same environment.

The crystal is built by placing an identical basis (the motif) on each of the lattice points.



Unit Cell

The building block of the crystal structure. Corners are lattice points. **Primitive** (contains 1 point) or **non-primitive**.





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Symmetry Operations

A crystal structure is "created" by replicating a motif with a variety of operations:

translations

■ rotation axes (symbols: 1,2,3,4,6 = nb of times the form is repeated in a 360° rotation)



inversion axes (combination of rotation and centre of symmetry operations)

Basics

The Bravais Lattices (14)



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The Space Groups (230)

All the symmetry operation on the 14 Bravais lattices. Describe the symmetry of the crystal system.

The Point Groups (32)

The Space Groups – the translations Describe the symmetry of the physical properties.

The Laüe Groups (11)

The Point Groups + a center of symmetry Describe the symmetry of the diffraction diagram.

Crystal structure

To draw a crystal structure, you need:

- the crystal system (define the arrangement of the lattice points)

- the lattice parameters (define the size and shape of the unit cell)

- the motif (groups of atoms) (the repeated unit at each lattice points)

Wurtzite structure



 $\begin{array}{l} Ga_1 \ (0, \ 0, \ 0) \\ N_1 \ \ (0, \ 0, \ 3/8) \\ Ga_2 \ (1/3, \ 2/3, \ 1/2) \\ N_2 \ \ (1/3, \ 2/3, \ 1/2+3/8 \) \end{array}$

Space Group: *P6*₃*mc*

Lattice planes

Miller indices

A method of describing the orientation of a plane in relation to the unit cell.

The plane (*hkl*) intercepts :

- x-axis at a/h
- y-axis at b/k
- z-axis at c/l

h, k, and I are integers.





Lattice vectors

A vector joining two lattice points.

A linear combination of the unit cell vectors (U, V and W are integers) :

 $\vec{R} = U\vec{a} + V\vec{b} + W\vec{c} \quad \iff \quad \vec{R} = \begin{bmatrix} UVW \end{bmatrix}$



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Crystallography conventions

How to write the indices of planes and directions?

- (*hkl*) a specific plane
- {*hkl*} a set of planes symmetrically equivalent
- [*UVW*] a specific vector or direction
- *<UVW>* a set of directions symmetrically equivalent

The 4-index notation or Miller-Bravais notation

For hexagonal lattice a 4-index notation can be used.

This notation possesses the apparent symmetry of the hexagonal lattice in the basal plane.

For plane notation: (*hkl*) \rightarrow (*hkil*) with *i* = -(*h*+*k*)



Basics









Direction notations

Directions in 4-index notation are less transparent in their construction.

$$\vec{R} = \begin{bmatrix} UVW \end{bmatrix} \qquad \longleftrightarrow \qquad \vec{R} = \begin{bmatrix} uvtw \end{bmatrix}$$

$$U = u - t \qquad \qquad u = (2U - V)/3$$

$$V = v - t \qquad \qquad v = (2V - U)/3$$

$$W = w \qquad \qquad t = -(u + v) = -(U + V)/3$$

$$w = W$$

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Basics



3-indices notation: **a**₁=[100] 4-indices notation? [1000] is not possible because $t \neq -(u+v)$ u = (2*1-0)/3 = 2/3v = (2*0-1)/3 = -1/3t = -(u+v) = -1/3w = 0u,v,t, w integers! **3a**₁=[2-1-10]

Interplanar spacing d_{hkl}

Miller indices define a family of parallel planes.

 d_{hkl} is referred to the distance between two successive (*hkl*) planes.



Basics



2. Diffraction or the reciprocal space

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Reciprocal lattice vector



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The reciprocal lattice

A reciprocal lattice vector can be defined from the reciprocal unit vectors :

$$\vec{d}_{hkl}^* = h\vec{a}^* + k\vec{b}^* + l\vec{c}^*$$

h, k, l are the Miller indices of the plane (hkl).

The reciprocal lattice points are indexed hkl with no brackets

The vector \vec{d}_{hkl}^* of the reciprocal lattice is normal to the (hkl) plane of the crystal lattice.

$$d_{hkl} = \frac{1}{\left| \vec{d}_{hkl}^* \right|}$$



Basics Reciprocal lattice



Basics Reciprocal lattice



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The Bragg's law

Constructive interference:

the path difference δ should be an integral number n of wavelengths λ .

 $\delta = AB + BC = 2dsin\theta$

$n\lambda = 2d\sin\theta$



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X-ray scattering

- X-rays are electromagnetic radiations (~1Å).
- Photons energy : $E = h \nu = hc / \lambda$ (~10keV).
- Interacts with atoms in many different ways : Compton, Auger, fluorescence and elastic scattering.
- Elastic scattering (or coherent scatter) \rightarrow structural information.

Elastic scattering

The electric field vector of x-rays vibrate the atomic charges.

X-ray electric field vector : $\vec{E} = \vec{E}_0 e^{j\omega t}$

• Scattered wave from an electron :

$$\vec{E}_e(\vec{r},t) = -r_e \frac{\vec{E}_0}{r} e^{j(\omega t - \vec{k}\vec{r})}$$

where r_e is the electron radius

Scattered wave from an atom :

where
$$f_i = \int \rho(\vec{m}) e^{j(\vec{k} - \vec{k}_0)\vec{m}} dv$$

the atomic scattering factor $\rho(\vec{m})$: the electronic density

$$\vec{E}_{at}(\vec{r},t) = \vec{E}_e(\vec{r},t).f_i$$

→ fa th

The atomic scattering factor increase with the atomic number : I (InN) > I (GaN)

 f_i is calculated for all atoms in the "International Tables for Crystallography" Vol C.

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Diffracted intensity from a crystal



- gives amplitude

- gives discrete peaks

 \vec{x}_i : atomic positions in the lattice \vec{T}_n : reciprocal lattice node positions $\vec{R} = h\vec{a}^* + k\vec{b}^* + l\vec{c}^*$

All wurtzite materials have the same kind of diffraction diagrams, the peak positions vary with a and c values.

Stereographic Projection



An imaginary line is drawn between an object in the northern hemisphere and the south pole (S).

In the projection diagram, the position of the object is shown at the point where the dashed line intersects the equatorial plane.



This projection allows to see the symmetry of the lattice.

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 $\varphi_{001} \implies \text{all } \varphi \text{ values}$

II. The 4-circles diffractometer

- 1. General overview
- 2. X-ray source
- 3. Primary optics
- 4. Sample stage
- 5. Secondary optics



The angles associated with the diffractometer movements:

- 3 sample's rotations: ω , ϕ , χ
- 1 detector's rotation: 2θ



X-ray laboratory source

Into an evacuated tube:

- electrons are emitted from a heated tungsten filament
- then accelerated by an electric potential (~40kV)
- to impinge on a metal target



Anode (target): Cu, Mo, Fe, Co, Cr.

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The anode is irradiated with a beam of high-energy electrons.

These electrons:

 loose energy when they arrived in the anode: this energy is transform into radiation.

 \rightarrow a broad band of continuous radiation (bremsstrahlung or white radiation)

 remove inner electron: allow electrons of high energy states to transfer to the vacant inner states.

→ the emission lines with well defined energies corresponding to electron transition of the atom: $K\alpha_1$, $K\alpha_2$, K_β .



Incident beam conditioning

The multilayer parabolic mirror



Figure 3.19. The principle of the multi-layer parabolic X-ray mirror. Λ_A and Λ_B are the periods at the extreme ends of the multi-layer mirror.



To obtain a parallel beam.

Small divergence into the vertical or the horizontal plane !

The monochromator





To obtain a monochromatic beam.

A single crystal of known orientation and *d*-spacing.

Following the Bragg law, each component wavelength of a polychromatic beam will be diffracted at a discrete angle.

Only the radiation of interest (K α_1) can go out the diffractometer $\pm \Delta \lambda$. $\Delta \lambda \rightarrow$ instrumental peak broadening.

High intensity cost.

Sample stage

3 translations:

• X,Y \rightarrow mapping

• Z \rightarrow to put the surface of the sample at the center of the diffractometer (ie the center of all the rotations ω , θ , ϕ , χ).

2 rotations:

 \rightarrow sample orientation: to put the normal of the atomic planes parallel to the φ -axis.







Secondary optics

- none (open detector)
- slits
- analyzer (or secondary-beam monochromator)

Detector

- single point
- line (1D) detector
- area (2D) detector (need 2D beam conditioning)

Diffraction geometries



Problem: low intensity and bad accuracy because of the vertical beam divergence

Solution: a χ angle become a ω angles by changing ϕ of 90°

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III. Diffraction from materials

- 1. Powder
- 2. Thin films
 - Phase identification
 - Layer thickness
 - Layer orientation
 - Lattice parameters
 - Alloy composition
 - Defects
- 3. Multilayers

Order in thin films



Amorphous: no order

Polycrystalline: many crystallites of varying orientation



Textured: the growth orientation is defined but several in plane orientation



Epitaxial: perfect registry with the orientation of the under layer

Powder diffraction

A powder is a polycrystalline material in which there are all possible orientations of the crystals.





The GaN powder diagram simulated with the CaRine software \rightarrow 20 values

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Thin films : phase and orientation

Epitaxial films: only the growth planes are in diffraction condition

Symmetric $2\theta/\omega$ scan



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Symmetric $2\theta = 2\omega$

Layer thickness



Symmetric $2\theta = 2\omega$

Symmetric $2\theta/\omega$ scan for a *hkl* reflection



GaN 002 2 θ/ω diagram simulated with the X'Pert Epitaxy software.

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Layer orientation

 ω -scans for a symmetric reflection with φ loop.



If at phi=180° the flat is perpendicular to the ω axis \rightarrow the tilt GaN / Si is parallel to the flat.

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Lattice parameters

Substrate: bulk lattice parameters

Layer:





or partially relaxed!

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Bragg law:
$$2d_{hkl}\sin\theta = \lambda$$

Where θ is the half part of the detector position ($\neq \omega$ be careful)

For hexagonal lattices:
$$d_{hkl} = \frac{1}{\sqrt{\frac{4}{3a^2} \left(h^2 + k^2 + hk\right) + \frac{l^2}{c^2}}}$$

At least 2 d_{hkl} are needed, with good choice of *hkl*.

$$d_{00l} = \frac{c}{l} \qquad \qquad d_{h00} = \frac{\sqrt{3}}{2} \frac{a}{h}$$

Example for *c*-plane GaN:

• Symmetric reflections are *001* reflections:

symmetric $2\theta/\omega$ scans $\rightarrow d_{OOI} \rightarrow c$ lattice parameter

• *h00* reflections are in-plane reflections: too weak intensities \rightarrow we can't measure directly the *a* lattice parameter!

• With the *c* value and one d_{hol} we can determine the *a* value.

 d_{hOl} is determined from asymmetric 20/ ω scans.



Accuracy versus intensity

The choice of the secondary optics depends on the diffracted intensity:

• slit:	high intensity, broad peak
 analyzer: 	low intensity, sharp peak

Sharper is the peak better is the accuracy of the θ value.



From the Bragg law:

 $\frac{\Delta d}{d} = \cot\theta \times \Delta\theta$

As $\cot\theta$ is decreasing from $\theta=0$ to $\theta=90^{\circ}$ *(hkl)* planes that diffract at high angles 2 θ are needed.

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Lattice parameters from RSM



An other method is to measure 2θ and ω .

 $\omega = \theta_{hkl} \pm \chi_{hkl}$

Asymmetric (*w* offset)



Reciprocal Space Map (RSM): a series of $2\theta/\omega$ scans at successive ω values.

 2θ and ω are converted into reciprocal lattice units s:

$$\left|\vec{S}\right| = \frac{1}{d_{hkl}} = \frac{2\sin\theta}{\lambda}$$

$$S_x = \frac{2}{\lambda} \sin \theta \sin \chi$$
 $S_z = \frac{2}{\lambda} \sin \theta \cos \chi$

Lattice parameters from RSM





Alloy composition

Vegard's rule:

The lattice parameters of an alloy vary linearly between the end members.

For a biaxial strain in a hexagonal system the out-of-plane strain is related to the in-plane strain by the C_{13} and C_{33} components of the elastic stiffness tensor :

$$\frac{c_{meas} - c_0}{c_0} = -\frac{2C_{13}}{C_{33}} \left(\frac{a_{meas} - a_0}{a_0} \right)$$

where c_{meas} and a_{meas} are the measured strained parameters c_0 and a_0 are the relaxed parameters

The elastic constants C_{13} and C_{33} are linearly interpolated between the values for the end members. A graphical method can be used to find the composition.

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Thin films : defects

GaN layers can be described as mosaic crystals characterized by both the mean size of the mosaic blocks and the mean angle of their rotation against each other.



The angles between the mosaic blocks are correlated with the densities of threading dislocations (TD).

The Williamson–Hall plots

For *c*-plane GaN layers:

- ω -scans of *OOI* reflections \rightarrow the tilt
- ω -scans of *h0l* reflections (skew geometry) \rightarrow the twist



 β is the FWHM of the ω -scan (rocking curve)

with open detector!

The slope = The tilt angle α

The interceptions with the ordinate \rightarrow The lateral correlation length L_{\parallel}

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Dislocation densities

002 and 302 ω -scans alloy to estimate tilt and twist:

 $\alpha_{\text{tilt}} = 0.5 \text{ x FWHM}_{0.02}$

Heinke et al., phys. stat. sol. (a) 176, 391 (1999) $\beta_{\text{twist}} = 1.14 \text{ x FWHM}_{302}$

Heinke et al., Appl. Phys. Lett. 77, 2145 (2000)

c-plane GaN films contain 3 types of threading dislocations with a line direction along [0001].

Each dislocation type is associated with a local lattice distortion:

- edge dislocations (b = 1/3 < 11 20 >) $\leftarrow \rightarrow$ lattice twist
- screw dislocations ($b = \langle 0001 \rangle$) $\leftarrow \rightarrow$ lattice tilt
- *mixed* dislocations (b = 1/3 < 11 23 >) $\leftarrow \rightarrow$ both

• If one assumes the TD are randomly distributed:

The screw dislocation density $N_{\rm screw}$:

$$N_{\rm screw} = \frac{\alpha_{\Omega}^2}{4.35 \times b_c^2}$$

where α_{Ω} is the tilt angle b_c is the Burgers vector of the screw-type TD

The edge dislocation density N_e :

$$N_e^{\text{rand}} = \frac{\beta^2}{4.35 \times b_e^2}$$

where β is the twist angle b_e is the Burgers vector of the edge-type TD

There are usually less than 2% screw dislocations but the ratio of mixed to edge dislocations is variable.

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Assuming a mosaic structure where dislocations are located at grain boundaries:



 $N_e^{\rm corr} = \frac{\beta}{2.1 \times b_e d_0}$

where d_0 is the grain diameter (=lateral correlation length)

FIG. 11. Edge-type TD densities as a function of the grain diameter as determined by TEM and XRD. Either a random [Eq. (2)] or a correlated [Eq. (3)] distribution of the TDs was assumed for evaluating the XRD data. The dashed line is a least-square fit of the TEM data.

Chierchia et al., J. Appl. Phys., Vol. 93, No. 11, 2003.



For each *hkl* reflection, a lot of "satellite" peaks:

- from the space between the satellites \rightarrow the superlattice period Λ
- from the position of the 0 order satellite \rightarrow the average composition of the bi layer (A+B)
- from the relative intensity \rightarrow A and B composition and thickness

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λ

 $\Delta(2\theta)\cos\theta$

 $\Lambda =$

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Period:
$$\Lambda = t_w + t_b = 18.9 nm$$

Average composition:

$$C_{In}^{ave} = C_{In} \times \frac{t_w}{\Lambda} = 4.2\%$$



$$C_{In} \times \frac{t_w}{18.9} = 4.2\%$$

 $t_{...} + t_{h} = 18.9$

for 3 variables t_w, t_b, C_{In}



Maybe the relative intensities could be useful?



Diffraction from materials Multilayers



 t_w and t_b are adjusted to fit C_{In}^{ave} and Λ

The relative intensities vary for the high order satellite peaks.

A peak with a minimum intensity is helpful!

Slit or analyzer?



The thickness fringes is a merit figure of the superlattice.

Both!

The slit allows to measure the weak high order satellite peaks.

The end

X-ray diffraction is a powerful tool to characterize the structure of ordered materials.

Pe	$\delta_3 m$	С
No.	186	



Patterson symmetry P6/mmm





Origin on 3m1 on 6, mc

 Asymmetric unit
 $0 \le x \le \frac{2}{5}$;
 $0 \le y \le \frac{1}{5}$;
 $0 \le z \le 1$;
 $x \le (1+y)/2$;
 $y \le x/2$

 Vertices
 $0, 0, 0 = \frac{1}{2}, 0, 0 = \frac{3}{2}, \frac{1}{5}, 0$ $0, 0, 1 = \frac{1}{2}, 0, 1 = \frac{2}{3}, \frac{1}{5}, 1$

Symmetry operations

(1)	1		(2) 3 ⁺ 0,0,z	(3) 3 ⁻ 0,0,z	
(4)	$2(0, 0, \frac{1}{2})$	0,0,z	(5) 6 ⁻ (0,0, 1) 0,0,z.	$(6) 6^+(0,0,\frac{1}{2}) 0$	0,0,z
(7)	$m = x, \bar{x}, z$		(8) m x, 2x, z	(9) $m 2x, x, z$	
10)	C X,X,Z		(11) $c = x, 0, z$	(12) c 0, y, z	

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7)

Positions					
Multiplicity, Coordinates Wyckoff letter,				Reflection conditions	
Site symmetry					General:
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	(2) $\bar{y}, x - y, z$ (5) $y, \bar{x} + y, z + \frac{1}{2}$ (8) $\bar{x} + y, y, z$ (11) $x - y, \bar{y}, z + \frac{1}{2}$	(3) x (6) x (9) x (12) x	$+y, \bar{x}, z$ $-y, x, z + \frac{1}{2}$ x - y, z $x - y, z + \frac{1}{2}$		$\begin{array}{l} hh\overline{2h}l: \ l=2n\\ 000l \ : \ l=2n \end{array}$
					Special: as above, plus
6 c .m. x,x,z	$x, 2x, z = 2\bar{x}, \bar{x}, z$	$\bar{x}, x, z + \frac{1}{2}$	\bar{x} , $2\bar{x}$, $z + \frac{1}{2}$	$2x, x, z + \frac{1}{2}$	no extra conditions
2 b 3m. $\frac{1}{2}, \frac{2}{3}, z$	$\frac{1}{3}, \frac{1}{3}, z + \frac{1}{2}$				hkil : l = 2n or $h - k = 3n + 1$ or $h - k = 3n + 2$
2 a 3m. 0,0,z	$0, 0, z + \frac{1}{2}$				hkil : $l = 2n$
Symmetry of special project	ctions				
Along [001] $p 6mm$ $\mathbf{a}' = \mathbf{a} \mathbf{b}' = \mathbf{b}$ Origin at 0, 0, z	Along [100] p $\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$ Origin at $x, 0, 1$	$\mathbf{b}' = \mathbf{c}$		Along [21 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ Origin at 2	0] $p 1 m 1$ $\mathbf{b}' = \frac{1}{2} \mathbf{c}$ $x, \frac{1}{2}x, 0$
Maximal non-isomorphic s	ubgroups				
I [2] $P6_{,11}(P6_{,1}, 173)$ [2] $P31c(159)$ [2] $P3m1(156)$ (3] $P2mc(Cmc2, 36)$	1; 2; 3; 4; 5; 6 1; 2; 3; 10; 11; 12 1; 2; 3; 7; 8; 9				
[3] P2, mc (Cmc2, 36) [3] P2, mc (Cmc2, 36) [3] P2, mc (Cmc2, 36)	1; 4; 8; 11				AIN
IIa none				a (Å) 3.112
IIb [3] $H6_3 mc$ (a ' = 3 a , b ' =	: 3b) (P6, cm, 185)			<i>c</i> (Å) 4.982
Maximal isomorphic subgr	oups of lowest index			c/a	1.601
IIc [3] $P6_{3}mc$ (c' = 3c) (186); [4] $P6_{3}mc$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' =$	2b) (186)		(1013	3) 31.64°
Minimal non-isomorphic su	ipergroups			$(11\bar{2})$	2) 58.01°
I [2] P6 ₃ /mmc(194) II [3] H6 ₃ mc(P6, cm, 185); [2] $P6mm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (183))		(101	i) 61.59°

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InN

3.54

5.705

1.612

31.81°

58.18°

61.75°

GaN

3.189

5.185

1.626

32.04°

58.41°

61.96°

Other broadening factors

$$\beta_{\rm m}^2 = \beta_{\rm o}^2 + \beta_{\rm d}^2 + \beta_{\alpha}^2 + \beta_{\varepsilon}^2 + \beta_{\rm L}^2 + \beta_{\rm r}^2$$



 $\beta_{\rm m}$ is the measured FWHM

 β_0 is the intrinsic rocking curve width of the crystal β_d is the instrumental broadening width

- $\beta_{\alpha} \leftarrow$ lattice *rotations* at dislocations (tilt or twist)
- $\beta_{\varepsilon} \leftarrow$ lattice *strain* at dislocations (microstrain)
- $\beta_{L} \leftarrow$ limited correlation lengths
- $\beta_r \leftarrow$ wafer curvature

 β_0 and β_d are usually small compared with the tilt and the twist (a few arcsec).

For relatively high dislocation density films, β_{α} (tilt or twist) dominates and can be used as a measure of dislocation densities.





Figure 4. Broadening in reciprocal space due to different types of defects; (a) tilt, twist and limited size and (b) microstrain and composition/strain gradients. A, C and D are measured in asymmetric (some in symmetric) geometry while B is only accessible in skew symmetric geometry (or sometimes in-plane geometry); B is directed out of the page; limited size and microstrain can also broaden peaks out of the page. Instrumental resolution is the limiting factor for broadening of experimental scans. Note that this is a two-dimensional representation of broadening that can occur in all three dimensions.

Rep. Prog. Phys. 72 (2009) 036502

M A Moram and M E Vickers

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Alloy composition in semi-polar films



New coordinate systems \rightarrow rotation of tensors Hooke's law \rightarrow a term of shear appears

Defects in non-polar and semipolar films

• non-polar and semipolar films contain additional defects such as: intrinsic (I_1 , I_2 and I_3) and extrinsic (E) basal plane stacking faults (BSFs).

• I_1 BSFs formed by the insertion of an atomic plane (1/2 [0001]), followed by a shift of 1/3<1-100>, are bounded by sessile partial dislocations and arise due to growth errors. Typically, around 90% of observed BSFs are I_1 -type, as these have the lowest formation energy.

• The 10–10 and 20–20 reflections will be broadened by I_1 and I_2 BSFs when analysed in the skew symmetric geometry, whereas the 30–30 reflections will not be affected.