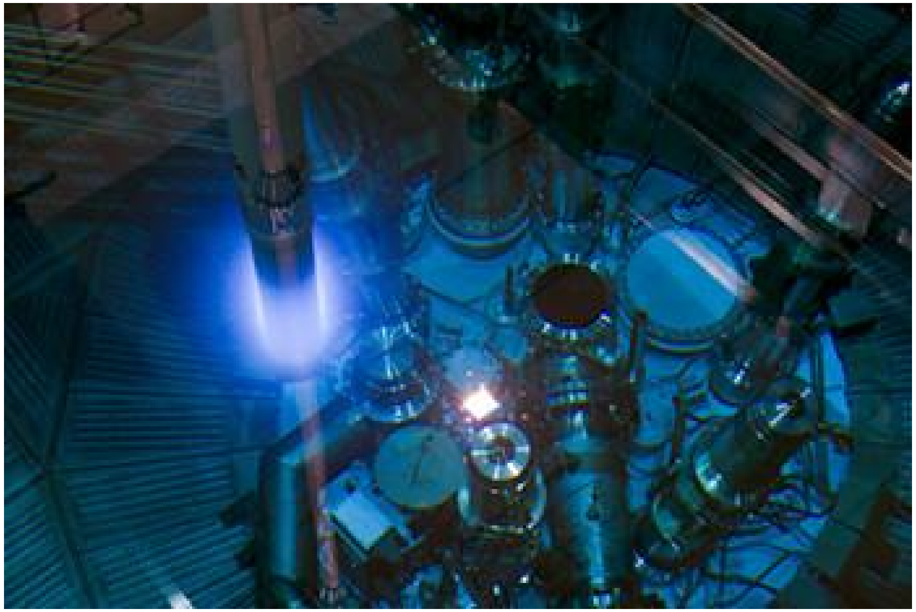
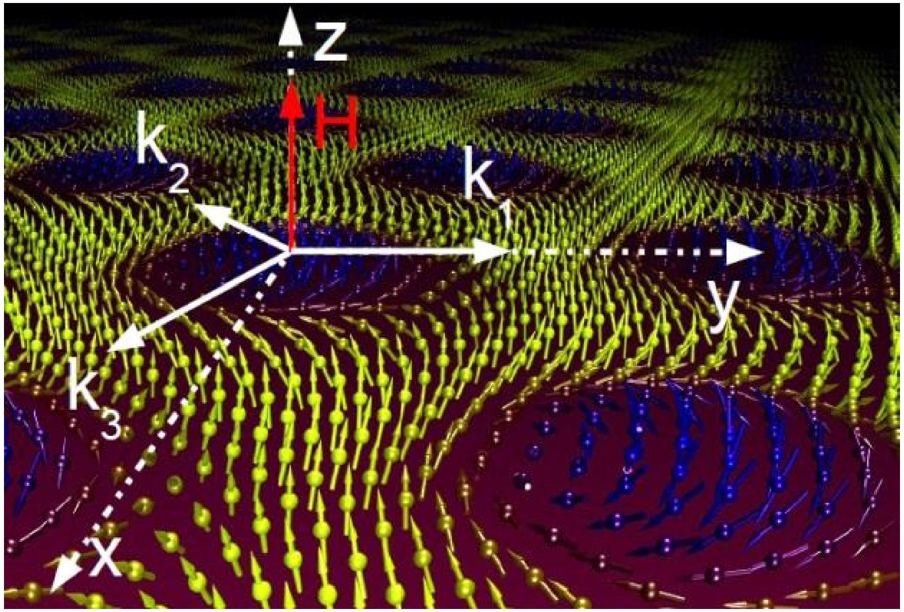
FRM II
Forschungs-Neutronenquelle
Heinz Maier-Leibnitz

MLZ
Heinz Maier-Leibnitz Zentrum

Physics with Neutrons I, WS 2015/2016





Lecture 7, 30.11.2015

MLZ is a cooperation between:

JÜLICH FORSCHUNGSZENTRUM

Helmholtz-Zentrum Geesthacht
Zentrum für Material- und Küstenforschung

TUM
Technische Universität München

Organization

Visit FRM II : 21.12.2015

10:15 – 13:00 (after the lecture)

Valid ID necessary!!!

Exam (after winter term)

- Registration: via TUM-Online between 16.11.2015 – 15.1.2015
- Email: sebastian.muehlbauer@frm2.tum.de for date arrangement
- 30min oral exam

3.3 Reminder: Coherent and incoherent scattering

Assume a large sample with statistically variations of b_j

No correlations among b: $\overline{b_{j'}b_j} = (\bar{b})^2, j' \neq j$

$$\overline{b_{j'}b_j} = (\overline{b^2}), j' = j$$

Double differential crosssection spilts up into two terms:

$$\left(\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega \mathrm{d}E'}\right)_{coherent} = \frac{\sigma_{coh.}}{4\pi}\frac{k'}{k}\frac{1}{2\pi\hbar}\sum_{j,j'}\int_{-\infty}^{\infty}\underline{\left\langle e^{i\kappa R_{j'}(0)}e^{-i\kappa R_j(t)}\right\rangle} e^{-i\omega t}\mathrm{d}t$$

$$\left(\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega \mathrm{d}E'}\right)_{incoherent} = \frac{\sigma_{inc.}}{4\pi}\frac{k'}{k}\frac{1}{2\pi\hbar}\sum_{j,j'}\int_{-\infty}^{\infty}\underline{\left\langle e^{i\kappa R_j(0)}e^{-i\kappa R_j(t)}\right\rangle} e^{-i\omega t}\mathrm{d}t$$

$$\sigma_{coh.} = 4\pi\bar{b}^2 \qquad \sigma_{inc.} = 4\pi(\overline{b^2} - \bar{b}^2)$$

3.3 Reminder: Coherent and incoherent scattering

Coherent

Spatial and temporal correlations between different atoms

- Interference effects:
- Given by average of b
  Bragg scattering

Incoherent

Spatial and temporal correlations between the same atom

- Constant in Q
- Given by variations in b due to spin, disorder, random atomic motion....

Reminder: 4.1 Elastic scattering from a single crystal

Final result for elastic coherent scattering on crystals

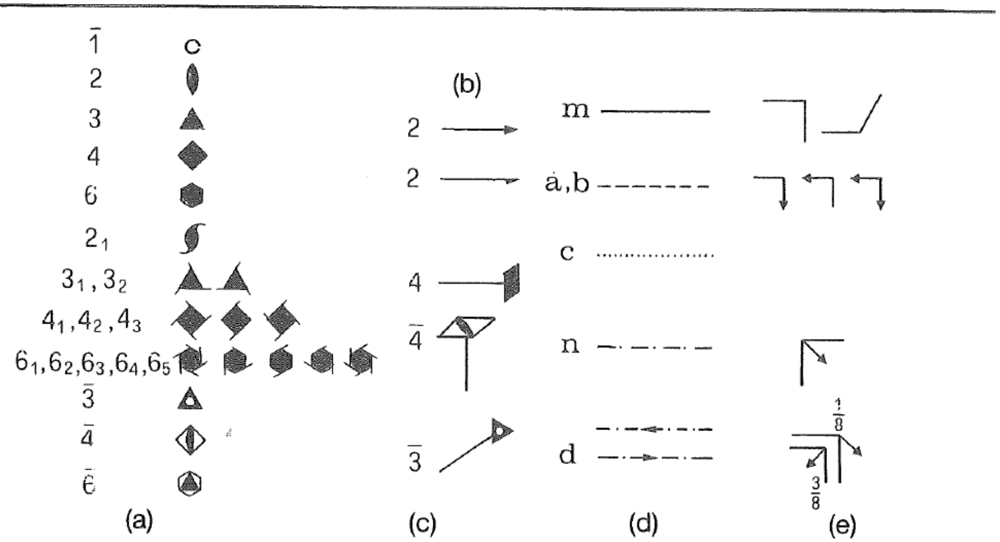
$$\frac{d\sigma}{d\Omega}_{coh.el} = N_0 \frac{(2\pi)^3}{v_0} e^{-2W(\vec{\kappa})} \sum_{\vec{\tau}} |S_{\vec{\tau}}|^2 \, \delta(\vec{\kappa} - \vec{\tau})$$

Normalization Debye-Waller Structure factor Bragg positions

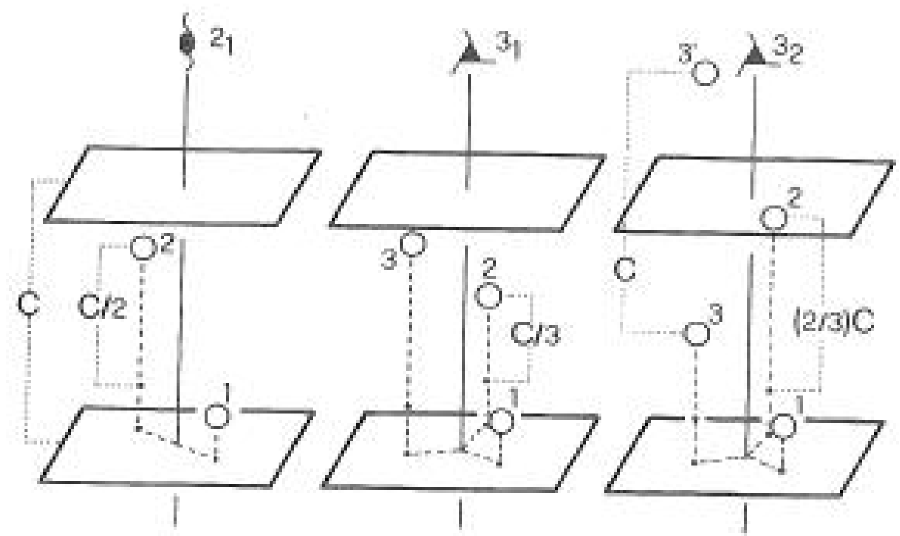
4.2 Appetizer Crystallography

Nomenclature rotation axes

Table 1.1. Graphical symbols for symmetry elements: (a) axes normal to the plane of projection; (b) axes 2 and 2_1 parallel to the plane of projection; (c) axes parallel or inclined to the plane of projection; (d) symmetry planes normal to the plane of projection; (e) symmetry planes parallel to the plane of projection

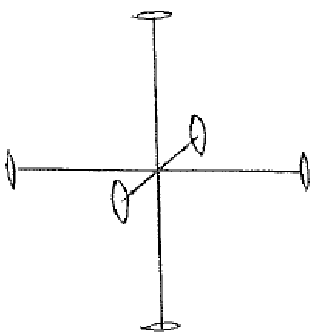


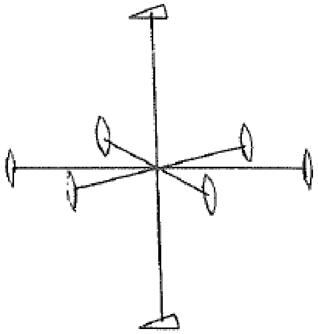
Examples: Screw axes

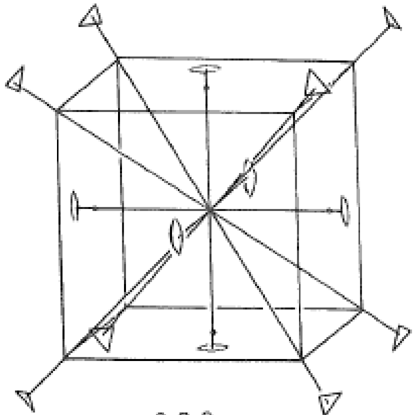


4.2 Appetizer Crystallography

Euler rules: Combination of roations





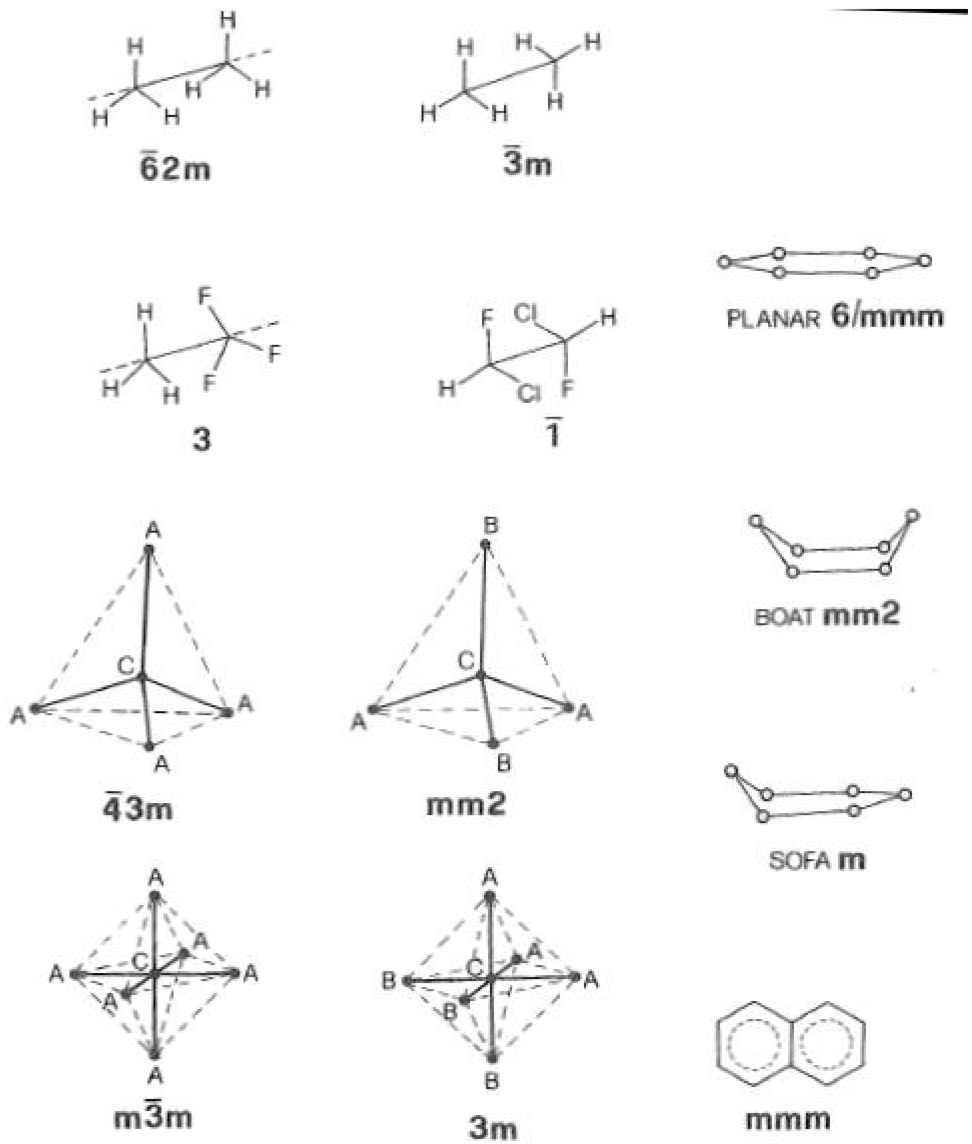


4.2 Appetizer Crystallography: 32 Point groups

Crystal systems	Point groups			Laue classes	Lattice point groups
	Non-centro-symmetric		Centro-symmetric		
Triclinic	1		$\bar{1}$	$\bar{1}$	$\bar{1}$
Monoclinic	2	m	2/m	2/m	2/m
Orthorhombic	222	mm2	mmm	mmm	mmm
Tetragonal	4	$\bar{4}$	4/m	4/m	4/mmm
	422	4mm, $\bar{4}$2m	4/mmm	4/mmm	
Trigonal	3		$\bar{3}$	$\bar{3}$	$\bar{3}$m
	32	3m	$\bar{3}$m	$\bar{3}$m	
Hexagonal	6	$\bar{6}$	6/m	6/m	6/mmm
	622	6mm, $\bar{6}$2m	6/mmm	6/mmm	
Cubic	23		m$\bar{3}$	m$\bar{3}$	m$\bar{3}$m
	432	$\bar{4}$3m	m$\bar{3}$m	m$\bar{3}$m	

4.2 Appetizer Crystallography

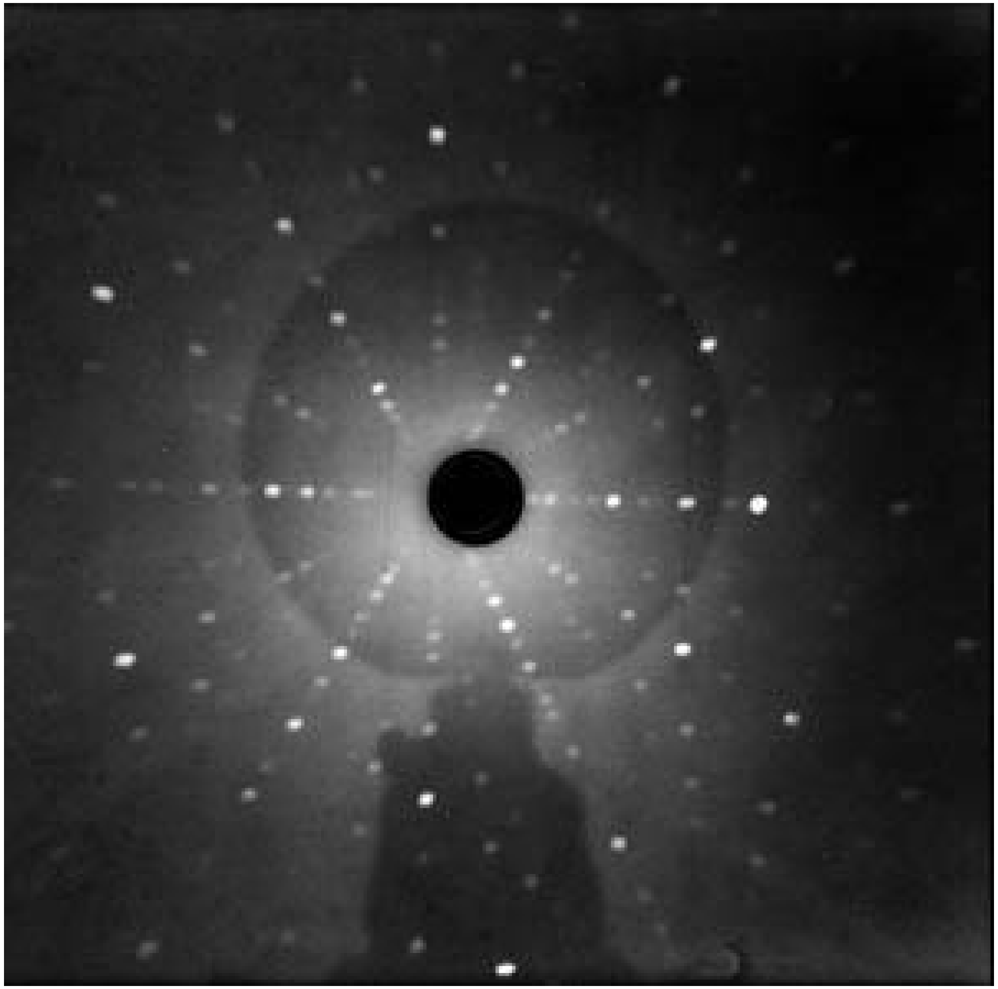
Point groups: examples



4.2 Appetizer Crystallography: Point groups & Laue classes

Crystal systems	Point groups: Non-centro-symmetric		Point groups: Centro-symmetric	Laue classes	Lattice point groups
Triclinic	1		$\bar{1}$	$\bar{1}$	$\bar{1}$
Monoclinic	2	m	2/m	2/m	2/m
Orthorhombic	222	mm2	mmm	mmm	mmm
Tetragonal	4	$\bar{4}$	4/m	4/m	4/mmm
	422	4mm, $\bar{4}$2m	4/mmm	4/mmm	
Trigonal	3		$\bar{3}$	$\bar{3}$	$\bar{3}$m
	32	3m	$\bar{3}$m	$\bar{3}$m	
Hexagonal	6	$\bar{6}$	6/m	6/m	6/mmm
	622	6mm, $\bar{6}$2m	6/mmm	6/mmm	
Cubic	23		m$\bar{3}$	m$\bar{3}$	m$\bar{3}$m
	432	$\bar{4}$3m	m$\bar{3}$m	m$\bar{3}$m	

4.2 Appetizer Crystallography: Laue classes, Friedels law



Laue forward scattering

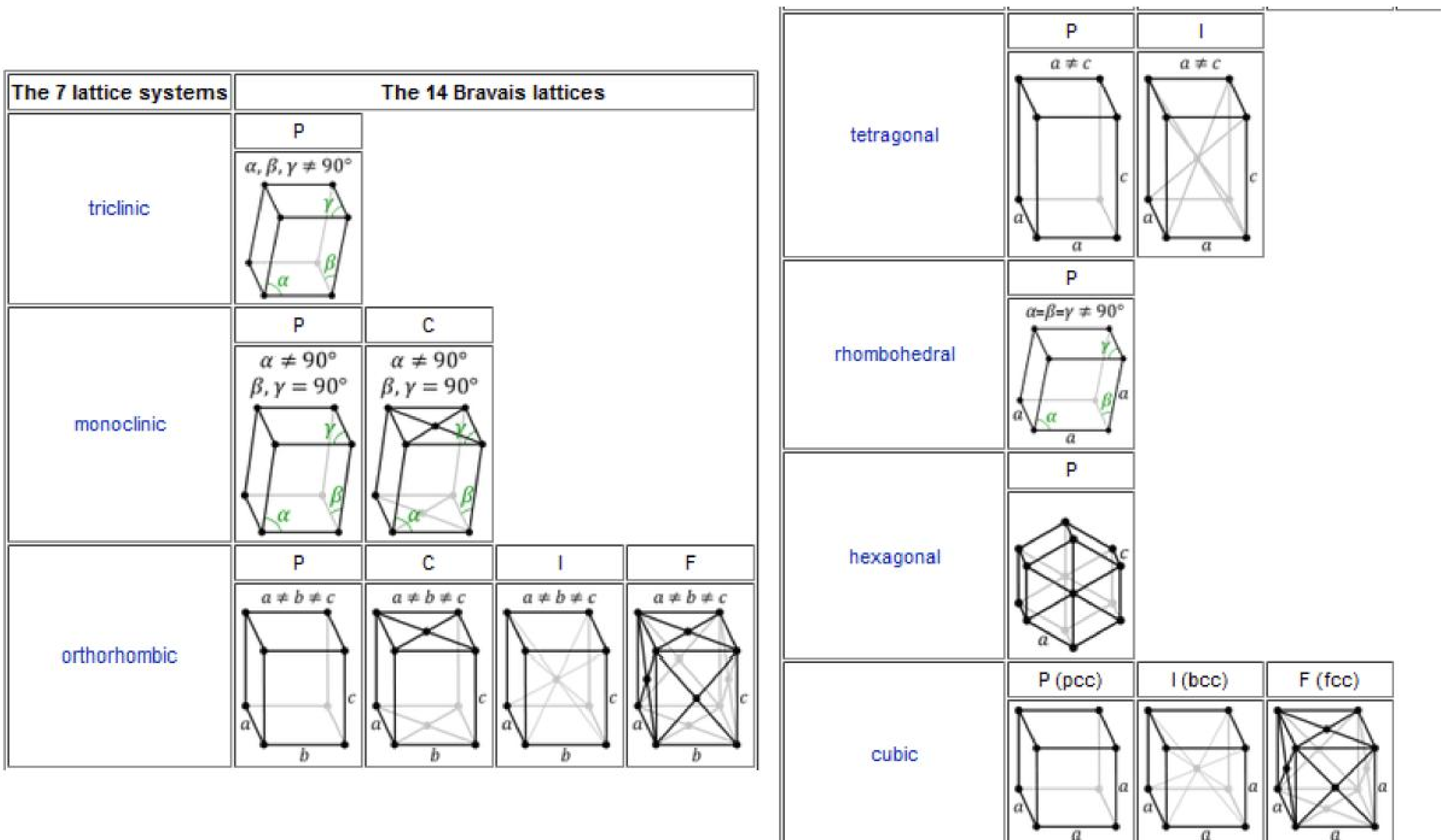
Silicon single crystal, cubic, fcc,
[111], three fold

4.2 Appetizer Crystallography: 7 crystal classes

Table 1.8. The conventional types of unit cell

Symbol	Type	Positions of additional lattice points	Number of lattice points per cell
P	primitive	—	1
I	body centred	(1/2, 1/2, 1, 2)	2
A	A-face centred	(0, 1/2, 1/2)	2
B	B-face centred	(1/2, 0, 1/2)	2
C	C-face centred	(1/2, 1/2, 0)	2
F	All faces centred	(1/2, 1/2, 0), (1/2, 0, 1/2)	2
		(0, 1/2, 1/2)	4
R	Rhombohedrally centred (de scription with 'hexagonal axes')	(1/3, 2/3, 2/3), (2/3, 1/3, 1/3)	3

4.2 Appetizer Crystallography: 14 Bravais Lattices



4.2 Appetizer Crystallography:

320 space groups

Table 1.9. The 230 three-dimensional space groups arranged by crystal systems and point groups. Space groups (and enantiomorphous pairs) that are uniquely determinable from the symmetry of the diffraction pattern and from systematic absences (see p. 159) are shown in bold-type. Point groups without inversion centres or mirror planes are emphasized by boxes

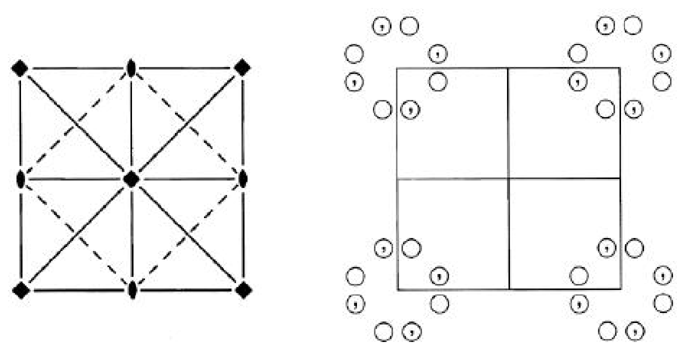
Crystal system	Point group	Space groups
Triclinic	$\boxed{1}$	$P1$
	$\bar{1}$	$P\bar{1}$
Monoclinic	$\boxed{2}$	$P2, P2_1, C2$
	m	Pm, Pc, Cm, Cc
	$2/m$	$P2/m, P2_1/m, C2/m, P2/c, P2_1/c, C2/c$
Orthorhombic	$\boxed{222}$	$P222, P222_1, P2_12_12, P2_12_12_1, C222_1, C222, F222, I222, I2_12_12_1$
	$mm2$	$Pmm2, Pmc2_1, Pcc2, Pma2_1, Pca2_1, Pnc2_1, Pmn2_1, Pba2, Pna2_1, Pnn2, Cmm2, Cmc2_1, Ccc2, Amm2, Abm2, Ama2, Aba2, Fmm2, Fdd2, Imm2, Iba2, Ima2$
	mmm	$Pmmm, Pnnn, Pccm, Pban, Pmma, Pnna, Pmna, Pcca, Pbam, Pccn, Pbcm, Pnnm, Pmmn, Pbcn, Pbca, Pnma, Cmcm, Cmca, Cmmm, Cccm, Cmma, Ccca, Fmmm, Fddd, Immm, Ibam, Ibca, Imma$
Tetragonal	$\boxed{4}$	$P4, P4_1, P4_2, P4_3, I4, I4_1$
	$\bar{4}$	$P\bar{4}, I\bar{4}$
	$4/m$	$P4/m, P4_2/m, P4/n, P4_2/n, I4/m, I4_1/a$
	$\boxed{422}$	$P422, P42_12, P4_122, P4_12_12, P4_222, P4_22_12, P4_322, P4_32_12, I422, I4_122$
	$4mm$	$P4mm, P4bm, P4_2cm, P4_2nm, P4cc, P4nc, P4_2mc, P4_2bc, I4mm, I4cm, I4_1md, I4_1cd$
	$\bar{4}m$	$P\bar{4}2m, P\bar{4}2c, P\bar{4}2_1m, P\bar{4}2_1c, P\bar{4}m2, P\bar{4}c2, P\bar{4}b2, P\bar{4}n2, I\bar{4}m2, I\bar{4}c2, I\bar{4}2m, I\bar{4}2d$
	$4/mmm$	$P4/mmm, P4/mcc, P4/nbm, P4/nnc, P4/mbm, P4/mnc, P4/nmm, P4/ncc, P4_2/mmc, P4_2/mcm, P4_2/nbc, P4_2/nnm, P4_2/mbc, P4_2mnm, P4_2/nmc, P4_2/ncm, I4/mmm, I4/mcm, I4_1/amd, I4_1/acd$
Trigonal–hexagonal	$\boxed{3}$	$P3, P3_1, P3_2, R3$
	$\bar{3}$	$P\bar{3}, R\bar{3}$
	$\boxed{32}$	$P312, P321, P3_112, P3_121, P3_212, P3_221, R32$
	$3m$	$P3m1, P31m, P3c1, P31c, R3m, R3c$
	$\bar{3}m$	$P\bar{3}1m, P\bar{3}1c, P\bar{3}m1, P\bar{3}c1, R\bar{3}m, R\bar{3}c$
	$\boxed{6}$	$P6, P6_1, P6_5, P6_3, P6_2, P6_4,$
	$\bar{6}$	$P\bar{6}$
	$6/m$	$P6/m, P6_3/m$
	$\boxed{622}$	$P622, P6_122, P6_522, P6_222, P6_422, P6_322$
	$6mm$	$P6mm, P6cc, P6_3cm, P6_3mc$
	$\bar{6}m$	$P\bar{6}m2, P\bar{6}c2, P\bar{6}2m, P\bar{6}2c$
	$6/mmm$	$P6/mmm, P6/mcc, P6_3/mcm, P6_3/mmc$
Cubic	$\boxed{23}$	$P23, F23, I23, P2_13, I2_13$
	$m\bar{3}$	$Pm\bar{3}, Pn\bar{3}, Fm\bar{3}, Fd\bar{3}, Im\bar{3}, Pa\bar{3}, Ia\bar{3}$
	$\boxed{432}$	$P432, P4_232, F432, F4_132, I432, P4_332, P4_132, I4_132$
	$\bar{4}3m$	$P\bar{4}3m, F\bar{4}3m, I\bar{4}3m, P\bar{4}3n, F\bar{4}3c, I\bar{4}3d$
	$m\bar{3}m$	$Pm\bar{3}m, Pn\bar{3}n, Pm\bar{3}n, Pn\bar{3}m, Fm\bar{3}m, Fm\bar{3}c, Fd\bar{3}m, Fd\bar{3}c, Im\bar{3}m, Ia\bar{3}d$

4.2 Appetizer Crystallography:

International tables of crystallography

$p4mm$ $4mm$

No. 11 $p4mm$ Pattersc



Origin at $4mm$

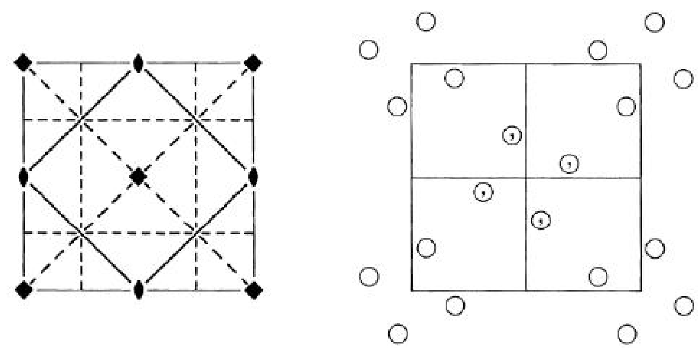
Asymmetric unit $0 \le x \le \frac{1}{2};\ 0 \le y \le \frac{1}{2};\ x \le y$

Symmetry operations

(1) x,y (2) $\bar{x},\bar{y}$ (3) $\bar{y},x$ (4) $y,\bar{x}$
(5) $\bar{x},y$ (6) $x,\bar{y}$ (7) y,x (8) $\bar{y},\bar{x}$

$4mm$ $p4gm$

Patterson symmetry $p4mm$ $p4gm$



Origin at $41g$

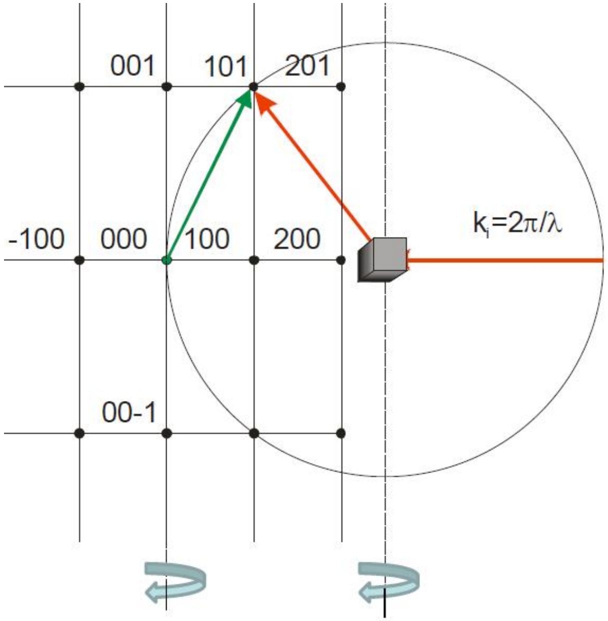
Asymmetric unit $0 \le x \le \frac{1}{2};\ 0 \le y \le \frac{1}{2};\ y \le \frac{1}{2}-x$

Symmetry operations

(1) x,y (2) $\bar{x},\bar{y}$ (3) $\bar{y},x$ (4) $y,\bar{x}$
(5) $\bar{x}+\frac{1}{2},y+\frac{1}{2}$ (6) $x+\frac{1}{2},\bar{y}+\frac{1}{2}$ (7) $y+\frac{1}{2},x+\frac{1}{2}$ (8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$

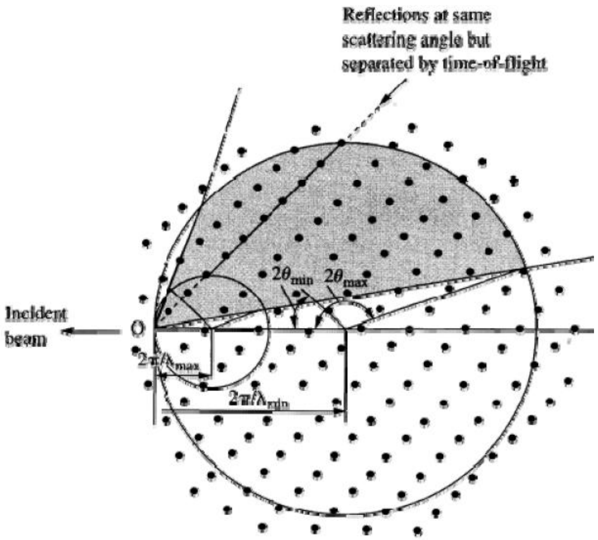
4.3 Diffraction: Monochromatic vs. TOF vs. Laue

Monochromatic beam



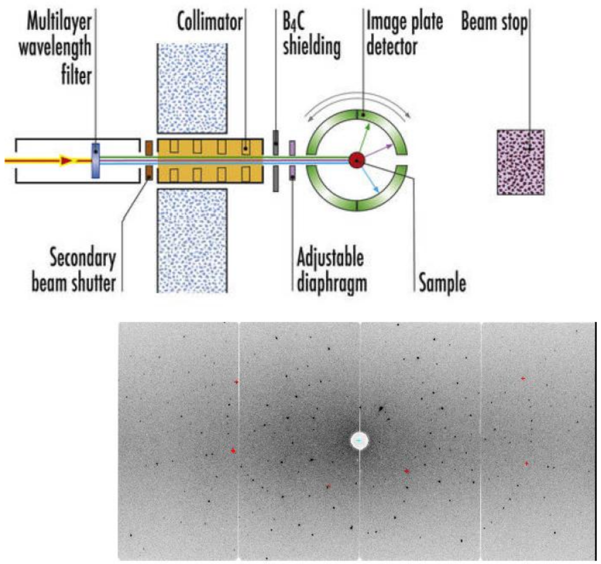
- Ewald construction
- Less intensity
- Rocking curve gives intensity of Bragg peak
- Clean data

Time-of-flight (TOF)



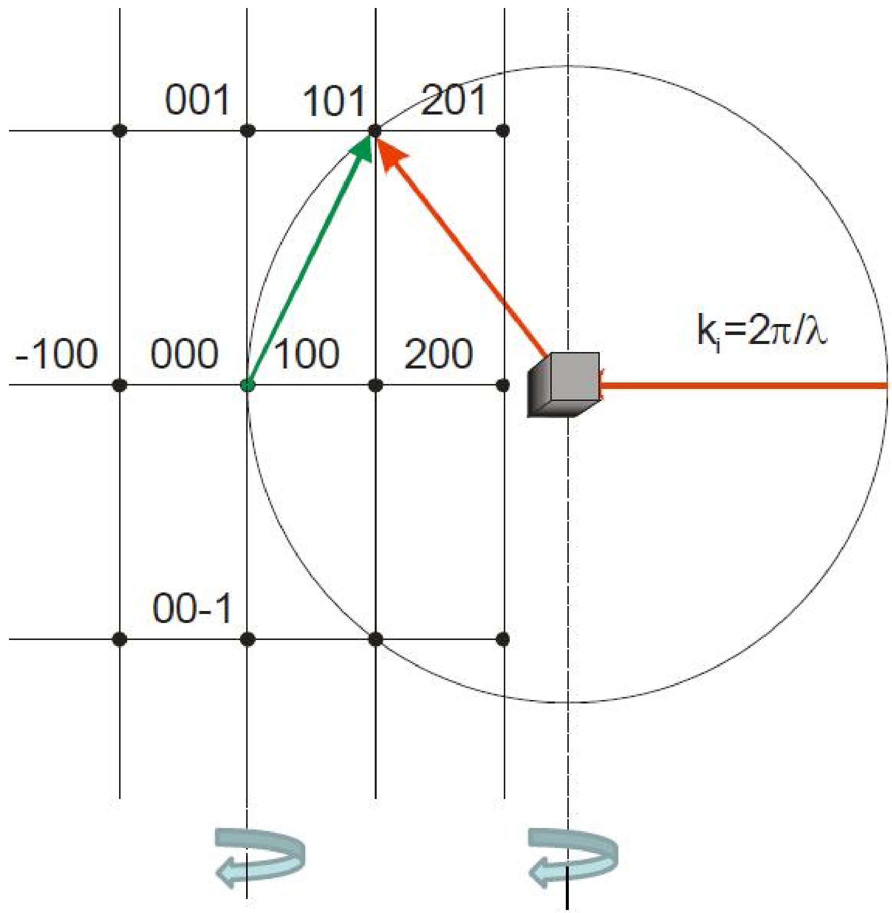
- Ewald construction for each wavelength in the beam
- Rocking curve distributed in time and detector
- Waste less neutrons

Laue (polychromatic beam)



- Essentially white beam
- More Bragg peaks (not stronger)
- Hard to get intensities
- Large background

4.3 Diffraction: Ewald construction for single crystal diffraction

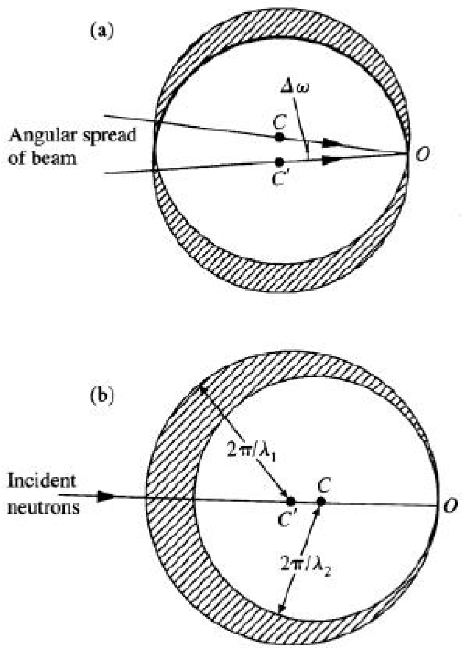


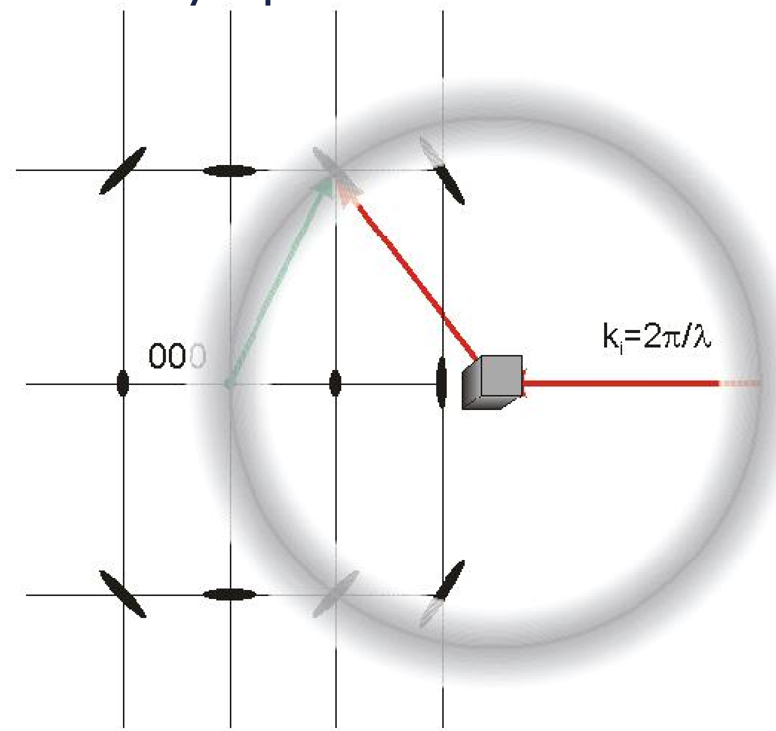
Ewald construction:

- Sphere around center of crystal (in real space)
- Origin of reciprocal space on transmitted beam at the edge of Ewald sphere
- Rotation of crystal (real space) corresponds to a rotation of reciprocal space

4.3 Diffraction: Ewald construction including resolution effects

- Mosaic spread of the sample (no perfect crystal)
- Finite spread of incoming beam (wavelength spread)
- Finite collimation of the incoming beam
  - Ewald construction for real samples: Fuzzy sphere





4.3 Diffraction: Crystal rotation method

- Solution: Measurement of **integrated intensity** and not **peak intensity**
- Fuzziness integrated out
  - Rocking scan