Components

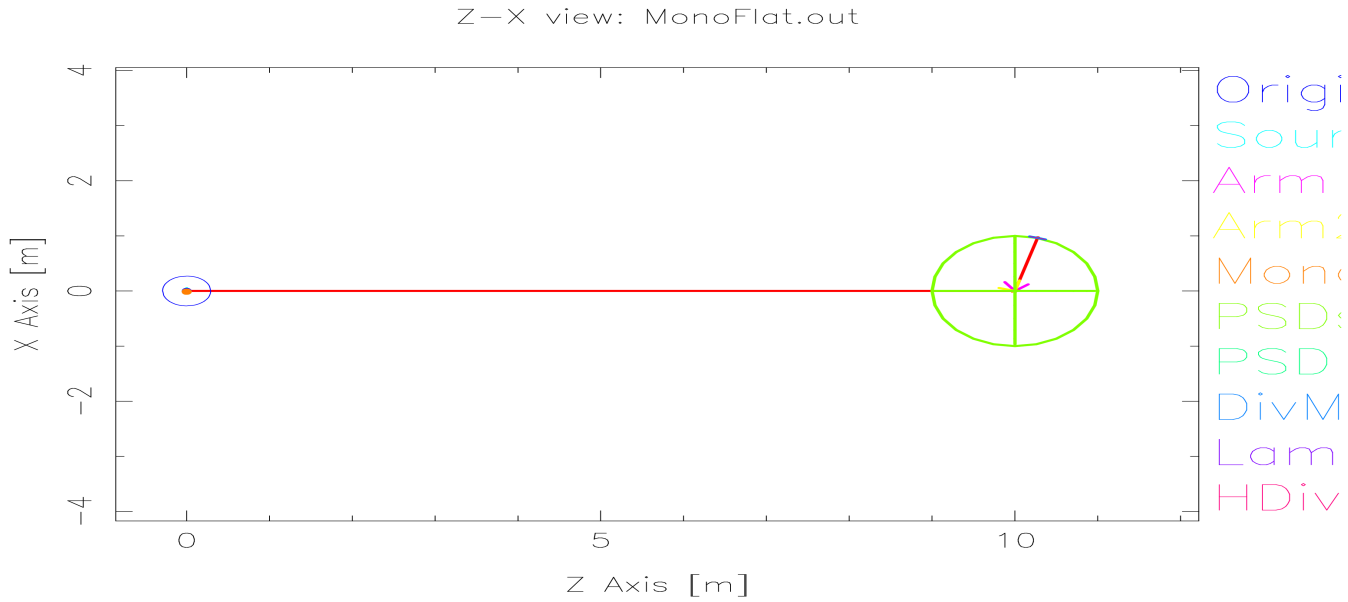
- Monochromator_flat (Ex 2.1.1)
- Monochromator_curved (Ex 2.1.2)
- Single_crystal (Ex 2.1.3)

Use in instrument

- Monochromator
- Analyser
- Sample

Build an instrument using

- `Source_simple` (0.1m*0.1m, dist=10, L0,dL, flat L distribution)
- Two `Arm` :one for rotation of mono and one for scattering
- `Monochromator_flat` (0.1m*0.1m @ z=10m, mosaic=40,r0=0.8,EXTEND if not scattered then absorb)
- `PSD_monitor`, `Divergence_monitor`, `L_monitor`



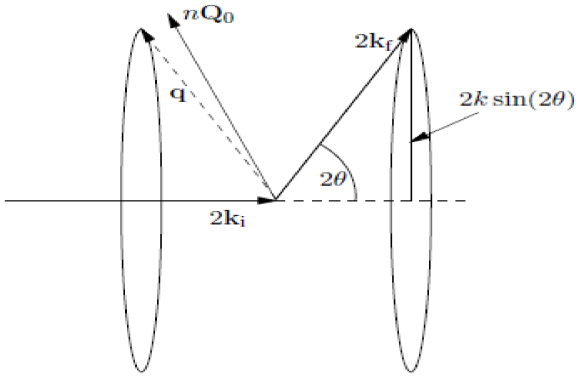
Properties:

- Infinitely thin, one scattering vector perpendicular to surface
  - no multiple scattering/secondary extinction
  - total reflectivity r0, not scattering cross sections
- Mosaic, vertical and horizontal η
- No variance of lattice parameter $\Delta d/d=0$

Algorithm:

- If intersect determine order n, $n\mathrm{Q}_0 = 2\mathrm{k}_i \sin\theta$
- From mosaicity η and angle α from Q_0 find prob $p_{\mathrm{reflect}} = R_0 e^{-\alpha^2/2\eta^2}$
- If reflected, determine direction on D-S cone
- Calculate weight for $\varphi \in [-\pi;\pi]$

$$f_{\mathrm{MC}}(\varphi) = \frac{1}{\sqrt{2\pi}(\alpha/\cos\theta)} e^{-\varphi^2/2(\alpha/\cos\theta)^2}$$



Input parameters

Parameters in **boldface** are required; the others are optional.

Name	Unit	Description	Default
zmin	m	Lower z-bound of crystal	0
zmax	m	Upper z-bound of crystal	0
ymin	m	Lower y-bound of crystal	0
ymax	m	Upper y-bound of crystal	0
width			0
height			0
mosaich	arc minutes	Horisontal mosaic (in Z direction) (FWHM)	30.0
mosaicv	arc minutes	Vertical mosaic (in Y direction) (FWHM)	30.0
r0	1	Maximum reflectivity	0.7
Q	AA-1	Magnitude of scattering vector	1.8734
DM	Angstrom	monochromator d-spacing instead of Q = 2*pi/DM	0

- `width = 0.1, height = 0.1,`
- `mosaich = MOSH, mosaicv = MOSV,`
- `r0 = 0.8, Q = 1.8734` (PG 002)

Basic setup

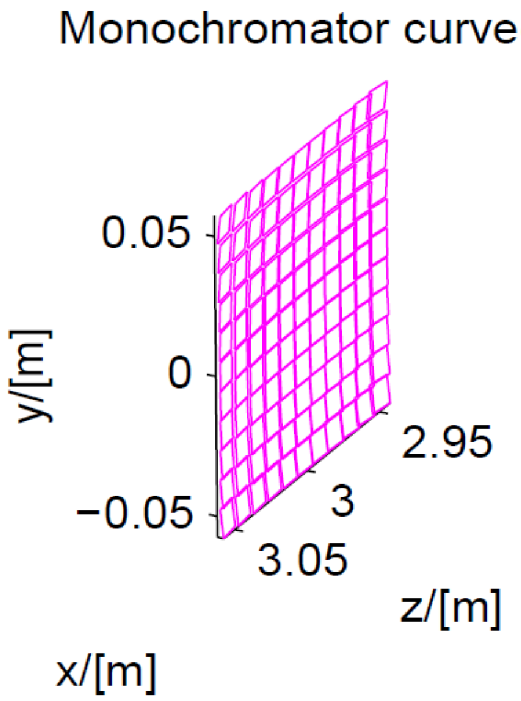
- Set source wavelength 4.0-4.1Å (`LMIN=4.0, LMAX=4.1`)
- Put mosaicity to 40 min (`MOSH=40, MOSV=40`)
- Set the monitors at the Bragg angle for the monochromator scattering for λ=4.045Å (rotate `a2`)
- Set monochromator rotation angle in scattering condition (`a1=a2/2`)
- Observe the wavelength distribution (n=1e6 rays is enough...)

Play!

- Try to put a broader wavelength interval from the source (2.0-4.1Å)
- Observe wavelength distribution
- Change to (vertical) mosaicity and observe the PSD
- Change the (horizontal) mosaicity and observe the energy monitor
- If you put a PSD_monitor_4PI (`radius=1-nm`) at the sample position you can confirm that only one scattering vector is present

Properties

- Array of single mosaic crystals (blades) with one scattering vector
- Infinitely thin, one scattering vector perp. to each surface of blade
  - no multiple scattering/secondary extinction
  - total reflectivity *r(k)*, not scattering cross sections
  - total transmission *t(k)*
- Mosaic, vertical and horizontal η
- No variance of lattice parameter $\Delta d/d=0$



Algorithm

For each individual blade the same as `Monochromator_flat`

Input parameters

Parameters in **boldface** are required; the others are optional.

Name	Unit	Description	Default
reflect	str	reflectivity file name of text file as 2 columns [k, R]	0
transmit	str	transmission file name of text file as 2 columns [k, T]	0
zwidth	m	horizontal width of an individual slab	0.01
yheight	m	vertical height of an individual slab	0.01
gap	m	typical gap between adjacent slabs	0.0005
NH	columns	number of slabs horizontal	11
NV	rows	number of slabs vertical	11
mosaich	arc minutes	Horisontal mosaic FWHM	30.0
mosaicv	arc minutes	Vertical mosaic FWHM	30.0
r0	1	Maximum reflectivity. 0 unactivates component	0.7
t0	1	transmission efficiency	1.0
Q	AA-1	Scattering vector	1.8734
RV	m	radius of vertical focussing. flat for 0	0
RH	m	radius of horizontal focussing. flat for 0	0
DM	Angstrom	monochromator d-spacing instead of Q=2*pi/DM	0
mosaic	arc minutes	sets mosaich=mosaicv	0
width	m	total width of monochromator	0
height	m	total height of monochromator	0
verbose	0/1	verbosity level	0

- 5 vertical slabs :`NV=5, yheight=0.02, zwidth=0.1, RV=1`
- Use reflecivity list '`HOPG.rfl`' provided in McStas datafiles
- Use transmission list '`HOPG.trm`' provided in McStas datafiles
- `r0 = 1,Q = 1.8734` (PG 002)

Basic setup

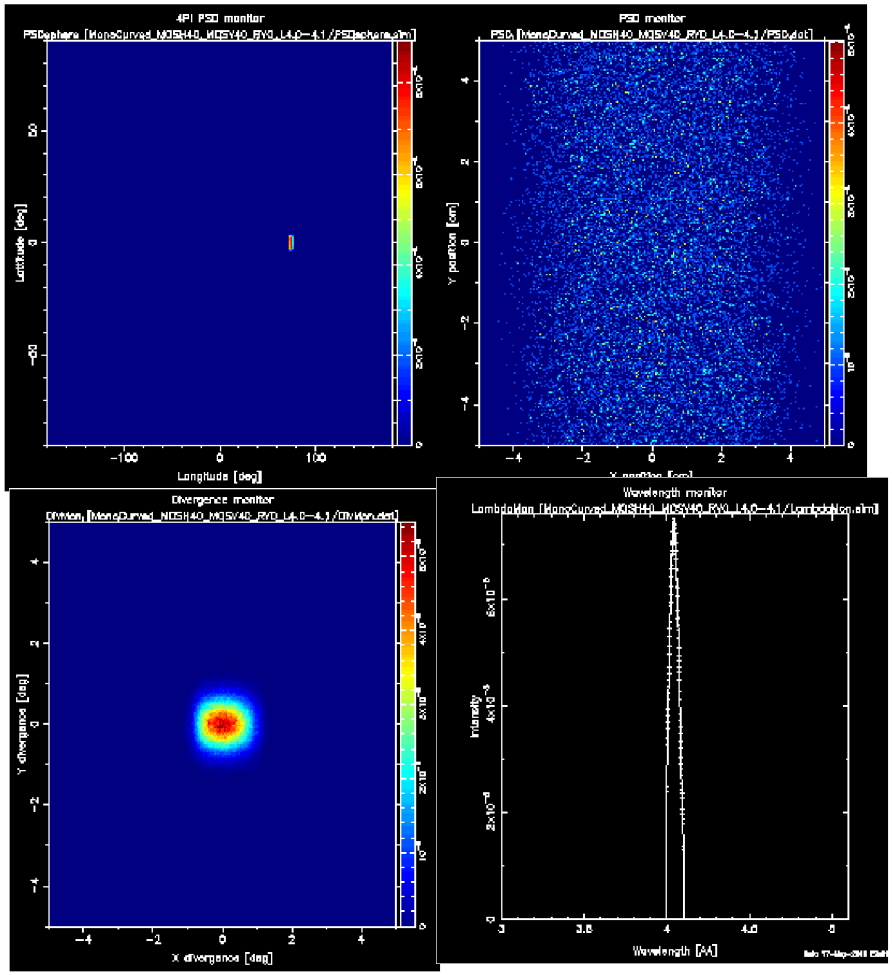
- Set source wavelength 4.0-4.1Å (`LMIN=4.0`, `LMAX=4.1`)
- Put mosaicity to 40 min (`MOSH=40`, `MOSV=40`)
- Set monochromator rotation angle `a1` in scattering condition
- Set the monitors `a2` at the Bragg angle for the monochromator scattering
- Observe the wavelength distribution (n=1e6 is enough...)

Play!

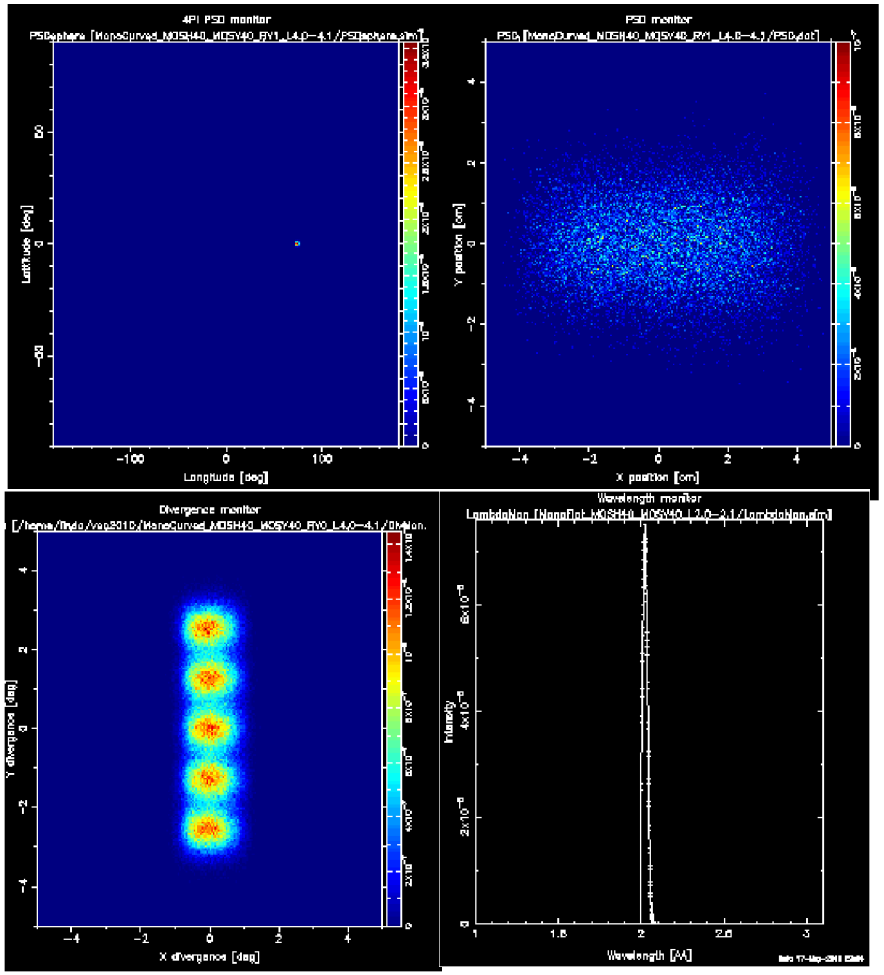
- Observe the influence of the focusing monochromator on the PSD (you can put it flat by setting `RV=0`)
- Observe the influence of the focusing monochromator on the divergence
- You can change the incoming wavelength (2.0-2.1 Å, second order scattering) and observe the intensity is smaller due to smaller reflectivity in comparison to constant r0

2.1.2: Monochromator_curved

No focus

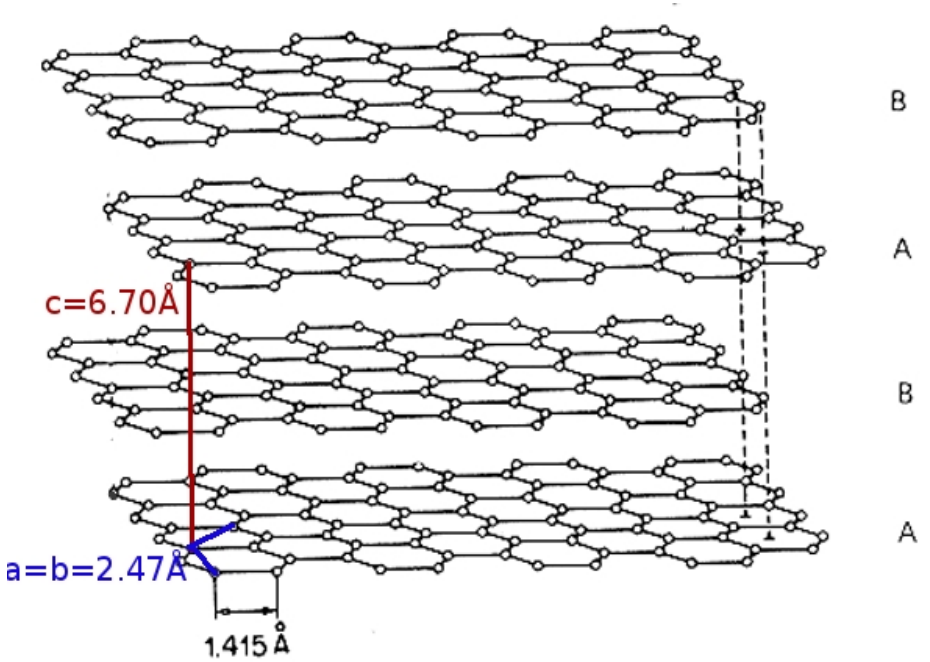


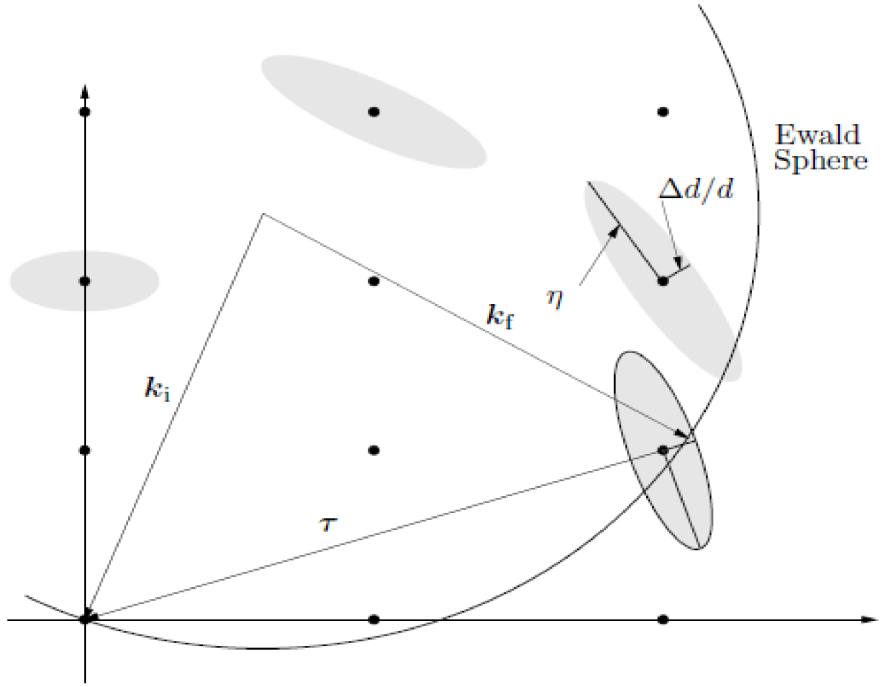
With focus



Properties

- Thick, flat single crystal
  - multiple scattering
  - absorption
- - incoherent scattering
- Mosaic, isotropic (anisotropic around sample lattice axes)
- Variance of lattice parameter $\Delta d/d$=0





Algorithm

The overview of the algorithm used in the Single_crystal component is as follows:

1. Check if the neutron intersects the crystal. If not, no action is taken.
2. Search through a list of reciprocal lattice points of interest, selecting those that are close enough to the Ewald sphere to have a non-vanishing scattering probability. From these, compute the total coherent cross-section σ_{coh} (see below), the absorption cross-section $\sigma_{\text{abs}} = \sigma_{2200}\frac{2200\ \text{m/s}}{v}$, and the total cross-section $\sigma_{\text{tot}} = \sigma_{\text{coh}} + \sigma_{\text{inc}} + \sigma_{\text{abs}}$.
3. The transmission probability is $\exp(-\frac{\sigma_{\text{tot}}}{V_0}\ell)$ where ℓ is the length of the flight path through the crystal. A Monte Carlo choice is performed to determine whether the neutron is transmitted. Optionally, the user may set a fixed Monte Carlo probability for the first scattering event, for example to boost the statistics for a weak reflection.
4. For non-transmission, the position at which the neutron will interact is selected from an exponential distribution. A Monte Carlo choice is made of whether to scatter coherently or incoherently. Absorption is treated by weight adjustment (see below).
5. For incoherent scattering, the outgoing wave vector $\boldsymbol{k}_{\text{f}}$ is selected with a random direction.
6. For coherent scattering, a reciprocal lattice vector is selected by a Monte Carlo choice, and $\boldsymbol{k}_{\text{f}}$ is found (see below).
7. Adjust the neutron weight as dictated by the Monte Carlo choices made.
8. Repeat from (2) until the neutron is transmitted (to simulate multiple scattering).

For point 2, the distance *dist* between a reciprocal lattice point and the Ewald sphere is considered small enough to allow scattering if it is less than five times the maximum axis of the Gaussian, $dist \leq 5\max(\sigma_1, \sigma_2, \sigma_3)$.

Input parameters

Parameters in **boldface** are required; the others are optional.

Name	Unit	Description	Default
reflections	string	File name containing structure factors of reflections. Use empty ("") or NULL for incoherent scattering only	
xwidth	m	Width of crystal	
yheight	m	Height of crystal	
zthick	m	Thichness of crystal (no extinction simulated)	
delta_d_d	1	Lattice spacing variance, gaussian RMS	1e-4
mosaic	arc minutes	Crystal mosaic (isotropic), gaussian RMS	-1
mosaic_h	arc minutes	Horizontal (rotation around Y) mosaic (anisotropic), gaussian RMS	-1
mosaic_v	arc minutes	Vertical (rotation around Z) mosaic (anisotropic), gaussian RMS	-1
mosaic_n	arc minutes	Out-of-plane (Rotation around X) mosaic (anisotropic), gaussian RMS	-1
recip_cell	1	Choice of direct/reciprocal (0/1) unit cell definition	0
ax	-		0
ay	AA or AA^-1	Coordinates of first (direct/recip) unit cell vector	0
az	-		0
bx	-		0
by	AA or AA^-1	Coordinates of second (direct/recip) unit cell vector	0
bz	-		0
cx	-		0
cy	AA or AA^-1	Coordinates of third (direct/recip) unit cell vector	0
cz	-		0
p_transmit	1	Monte Carlo probability for neutrons to be transmitted without any scattering. Used to improve statistics from weak reflections	-1
absorption	barns	Absorption cross-section per unit cell at 2200 m/s	0
incoherent	barns	Incoherent scattering cross-section per unit cell	0
aa	deg	.	0
bb	deg	unit cell angles alpha, beta and gamma. Then uses norms of vectors a,b and c as lattice parameters	0
cc	deg	.	0
order	1	limit multiple scattering up to given order (0: all, 1: first, 2: second, ...)	0
powder			0

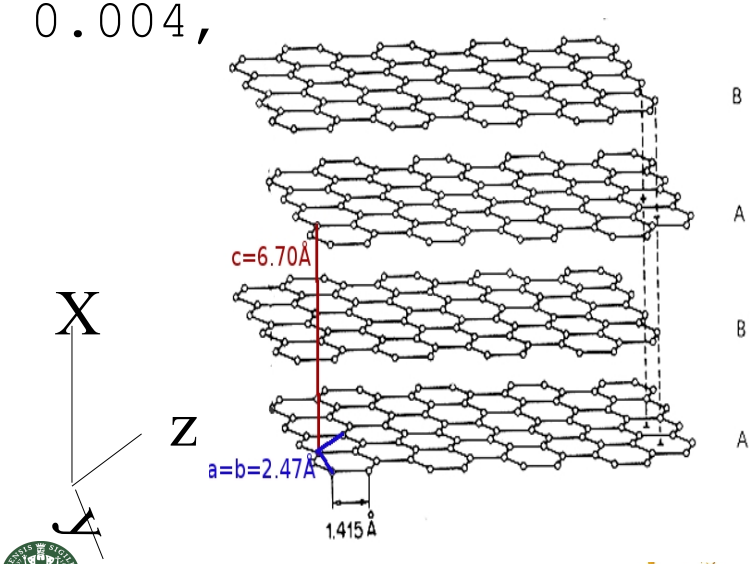
Basic setup

- A 2mm slab 0.1m*0.1m, small variance of lattice par, var. mos.:
  `xwidth = 0.002, yheight = 0.1, zthick = 0.1,`
  `delta_d_d = 1e-4, mosaic = MOS`
- Put the crystal with c axis along x, and b axis along z:
  `ax = 0, ay = 2.14, az = -1.24,` ($\alpha = 120$ deg)
  `bx = 0, by = 0, bz = 2.47,`
  `cx = 6.71, cy = 0, cz = 0,`
- Set the right reflection list (h k l F^2 [barns]) for graphite
  `reflections = "Graphite_long.dat",`
- σ_{abs}, σ_{inc} [barns] for graphite
  `absorption = 0.014, incoherent = 0.004,`
- Multiple scattering `order = 0` (all)

•Set monochromator rotation angle `a1` in scattering condition

• Set the monitors `a2` at the Bragg angle for the monochromator scattering

• Using wavelength 4.0-4.1Å you should get the same Bragg spot as before

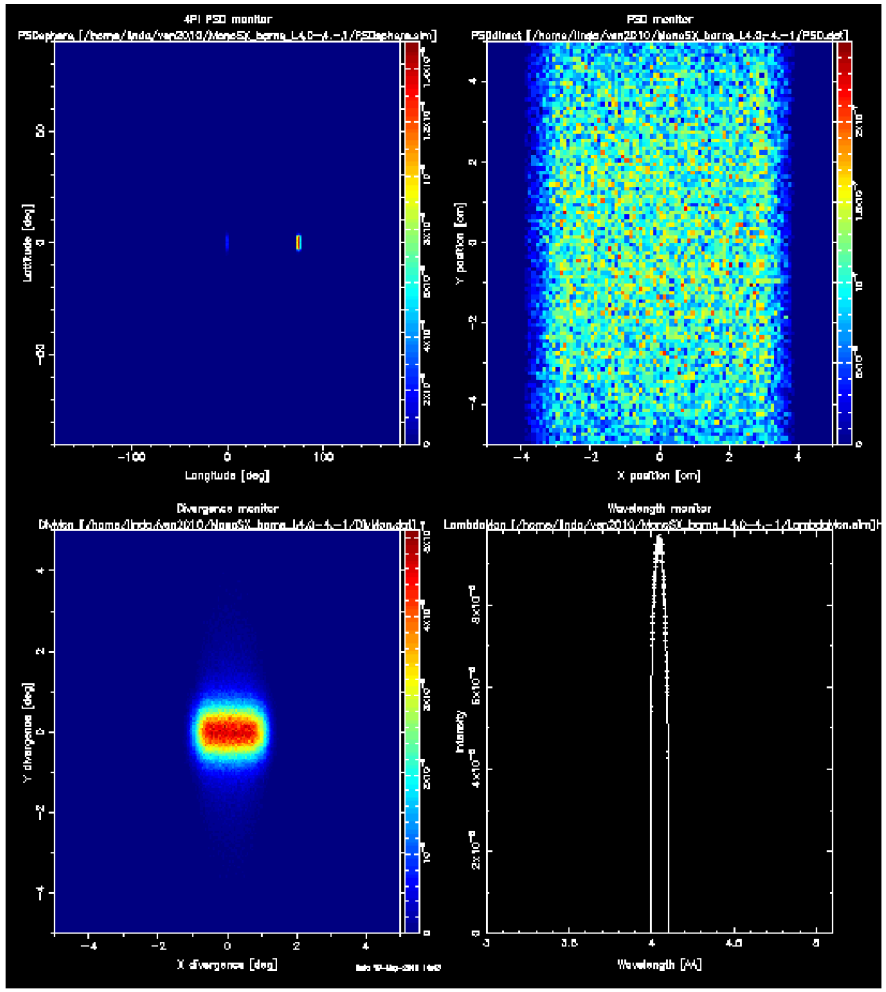


Play!

- Set a broader wavelength band from the source (2.1-4.1 Å)
- Observe the many reflections on the 4π PSD! (use log-scale)
  -this is why we need monochromator shielding :)
- You can also increase the incoherent scattering or absorption crosssection to observe the effect
- Or with the mosaicity or variance of latticespacing

2.1.3: Single_crystal

λ=4.0-4.1Å



λ=2.1-4.1Å