

Tuesday afternoon



Monochromators (Reactor track)

Presenter: Emmanuel Farhi



Monochromators

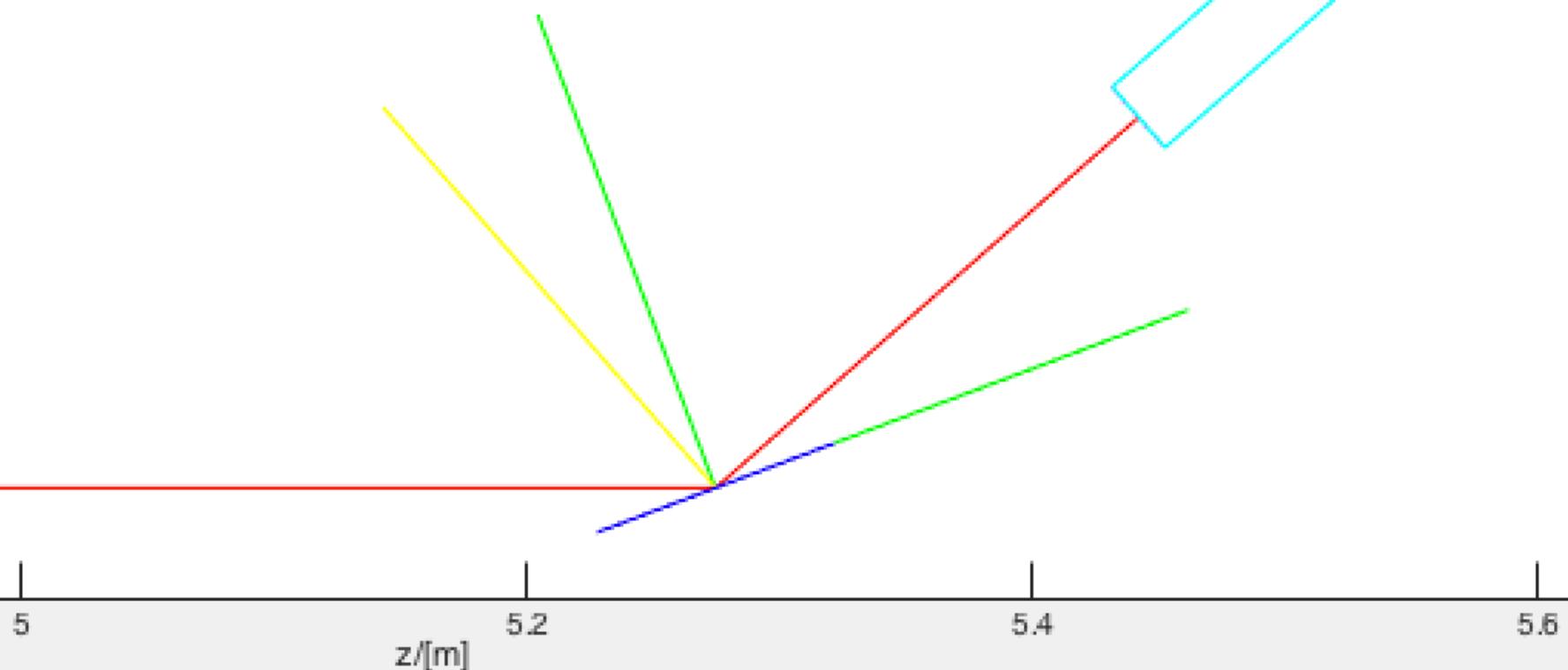
Components

- *Monochromator_flat*
- *Monochromator_curved*
- *Single_crystal*

Use in instrument

- *Monochromator*
- *Analyser*
- *Sample*

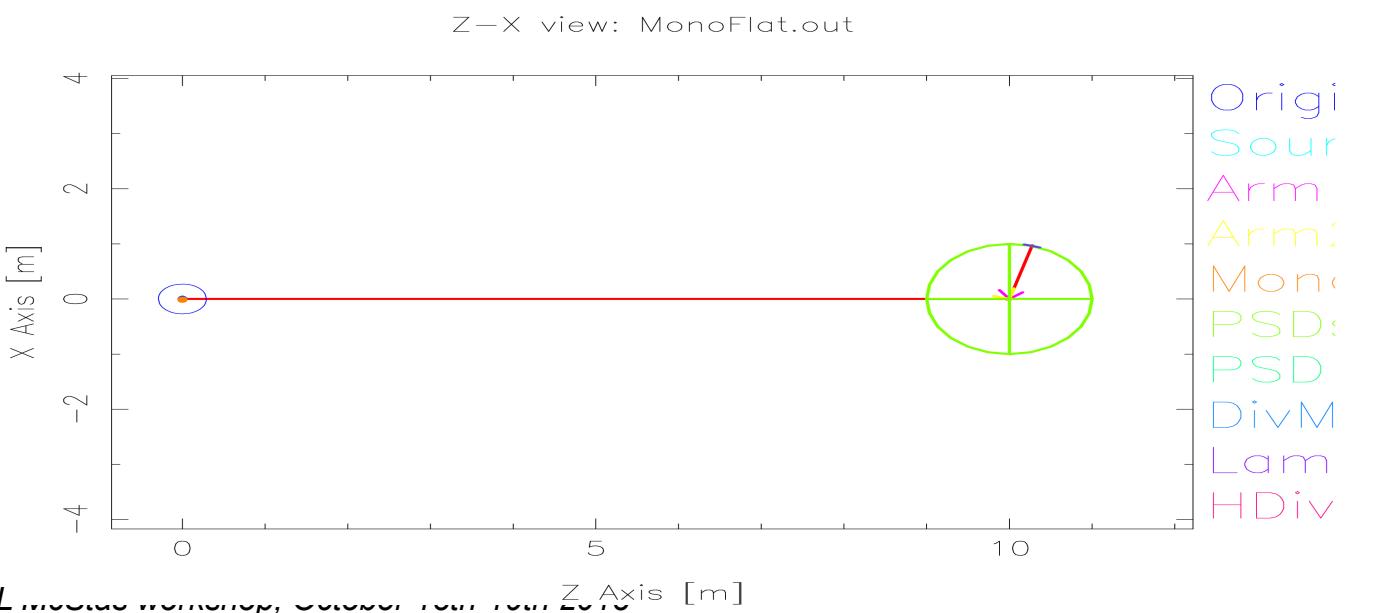
Quick step to the side: Arm()'s



Monochromator_flat

Build an instrument using

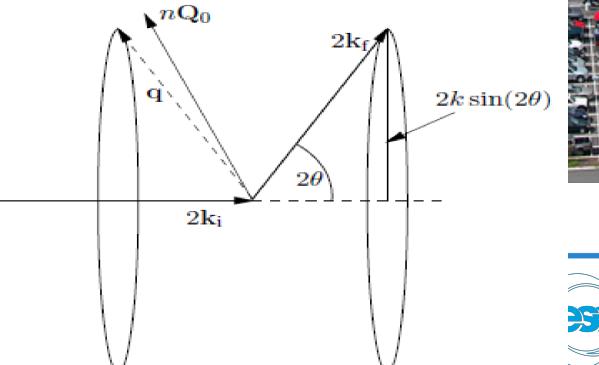
- *Source_simple (0.1m*0.1m, dist=10, lambda0,dlambda, flat wavelength distribution)*
- *Two Arm's: one for rotation of mono and one for scattering*
- *Monochromator_flat (0.1m*0.1m @ z=10m, from source mosaic=40,r0=0.8, (EXTEND if not scattered then absorb)*
- *PSD_monitor, Divergence_monitor, L_monitor*



Ven 2010



$$p_{\text{reflect}} = R_0 e^{-\alpha^2/2\eta^2}$$



Monochromator_flat

Properties:

- Infinitely thin, one scattering vector perpendicular to surface
 - no multiple scattering/secondary extinction
 - total reflectivity r_0 , not scattering cross sections
- Mosaic, vertical and horizontal η
- No variance of lattice parameter $\Delta d/d=0$

Algorithm:

- If intersect determine order n , $nQ_0 = 2k_i \sin \theta$

From mosaicity η and angle α from Q_0 find prob

- If reflected, determine direction on D-S cone
- Calculate weight for $\varphi \in [-\pi; \pi]$

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

Monochromator_flat ([link](#))

Input parameters

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

Name	Unit	Description	Default
zmin	m	Lower horizontal (z) bound of crystal	-0.05
zmax	m	Upper horizontal (z) bound of crystal	0.05
ymin	m	Lower vertical (y) bound of crystal	-0.05
ymax	m	Upper vertical (y) bound of crystal	0.05
zwidth	m	Width of crystal, instead of zmin and zmax	0
yheight	m	Height of crystal, instead of ymin and ymax	0
mosaich	arc minutes	Horizontal 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	1/angstrom	Magnitude of scattering vector	1.8734
DM	angstrom	monochromator d-spacing, instead of $Q = 2\pi/DM$	0

- $xwidth = 0.1$, $yheight = 0.1$,
- $mosaich = MOSH$, $mosaicv = MOSV$,
- $r0 = 0.8$, $Q = 1.8734$ (PG 002)



Monochromator_flat

Basic setup of the instrument file

- Set source wavelength $4.0\text{-}4.1\text{\AA}$ ($LMIN=4.0$, $LMAX=4.1$)
- Put mosaicity to 40 min ($MOSH=40$, $MOSV=40$)
- Set the monitors at the Bragg angle for the monochromator scattering for $\lambda=4.045\text{\AA}$ (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 ($2.0\text{-}4.1\text{\AA}$)
- 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* ($radius=1\text{-}nm$) at the sample

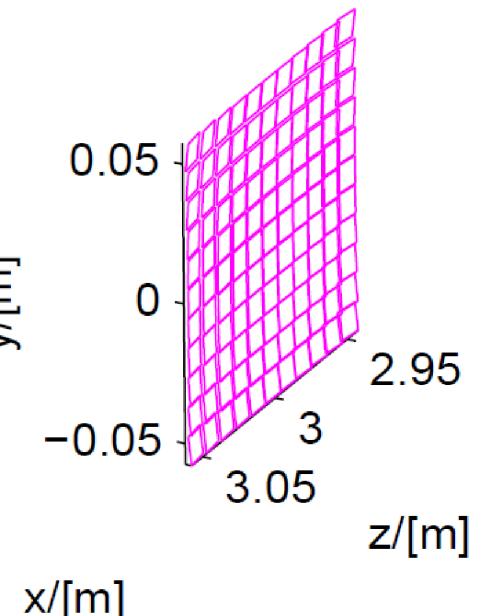


Monochromator_curved

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 $\Delta d/d = 0$*

Monochromator curved



Algorithm

For each individual blade the same as Monochromator flat

Monochromator curved ([link](#))

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]	"NULL"
transmit	str	transmission file name of text file as 2 columns [k, T]	"NULL"
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, along Z	0
height	m	total height of monochromator, along Y	0
verbose	0/1	verbosity level	0
order	1	specify the diffraction order, 1 is usually prefered. Use 0 for all	0



- *5 vertical slabs :NV=5, yheight=0.02, zwidth=0.1, RV=1*
- *Use reflectivity list 'HOPG.rf1' provided in McStas datafiles*
- *Use transmission list 'HOPG.trm' provided in McStas datafiles*
- *r0 = 1, Q = 1.8734 (PG 002)*

Monochromator_curved

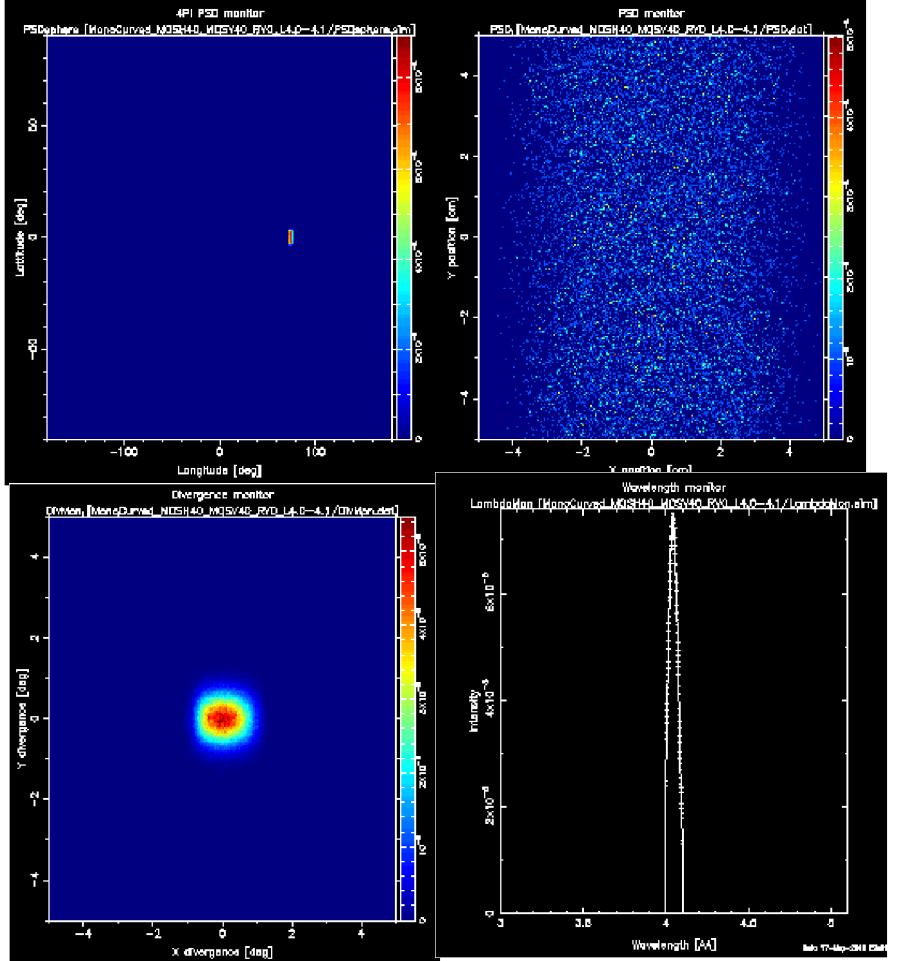
Basic setup of the instrument

- Set source wavelength $4.0\text{-}4.1\text{\AA}$ ($L_{MIN}=4.0$, $L_{MAX}=4.1$)
- Put mosaicity to 40 min ($MOSH=40$, $MOSV=40$)
- Set monochromator rotation angle α_1 in scattering condition
- Set the monitors α_2 at the Bragg angle for the monochromator scattering
- Observe the wavelength distribution ($n=1e6$ is enough...)
- 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 ($2.0\text{-}2.1\text{\AA}$, second order scattering) and observe the intensity is smaller due to smaller reflectivity in comparison to constant r_0

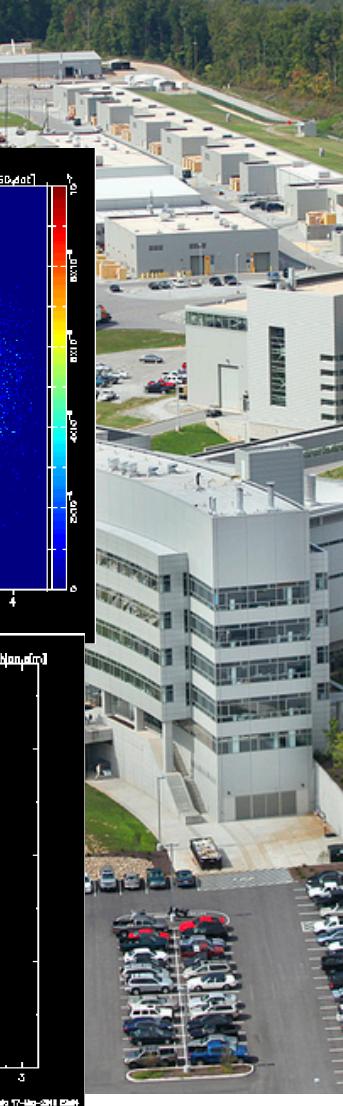
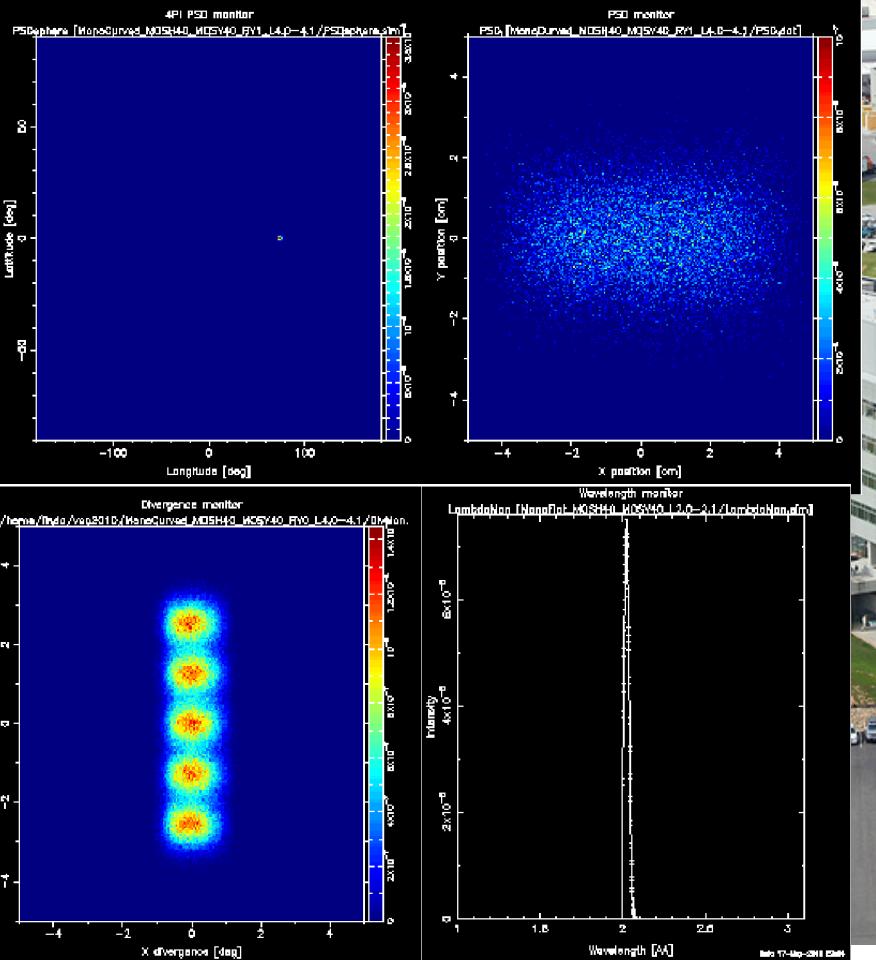


Monochromator_curved

No focus



With focus

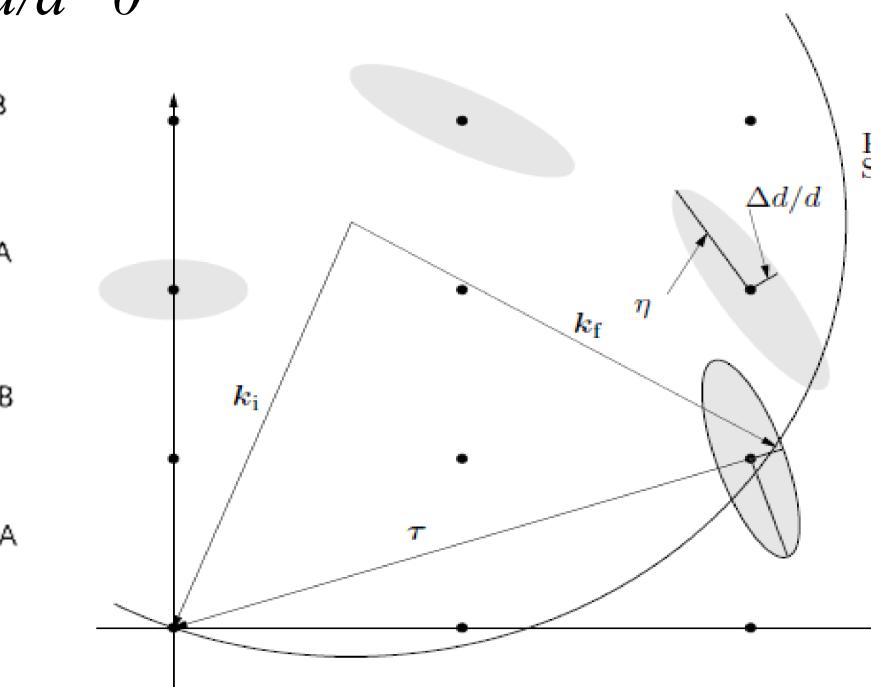
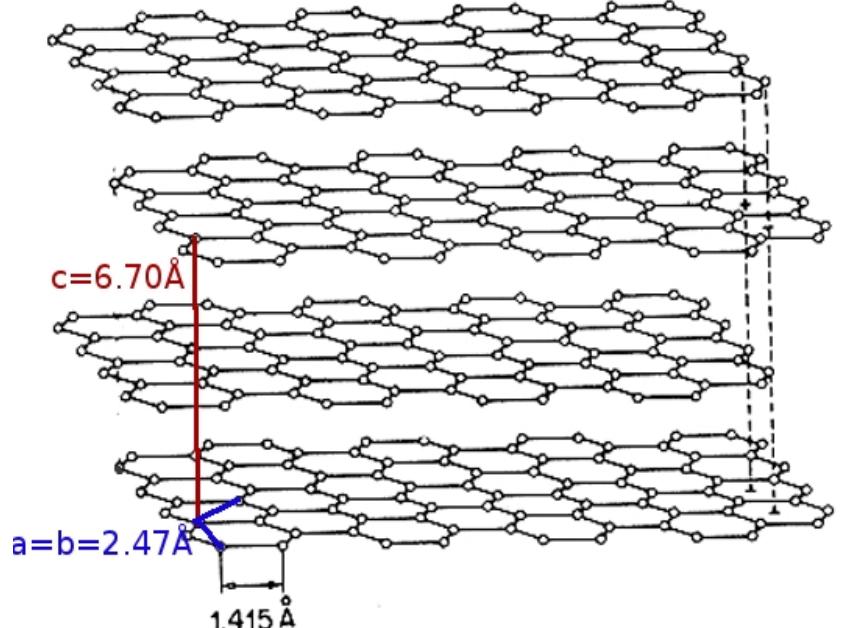




Single_crystal

Properties

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



Single_crystal - 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 k_f is selected with a random direction.
6. For coherent scattering, a reciprocal lattice vector is selected by a Monte Carlo choice, and k_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, $dist \leq 5 \max(\sigma_1, \sigma_2, \sigma_3)$.



Single_crystal ([link](#))

Input parameters

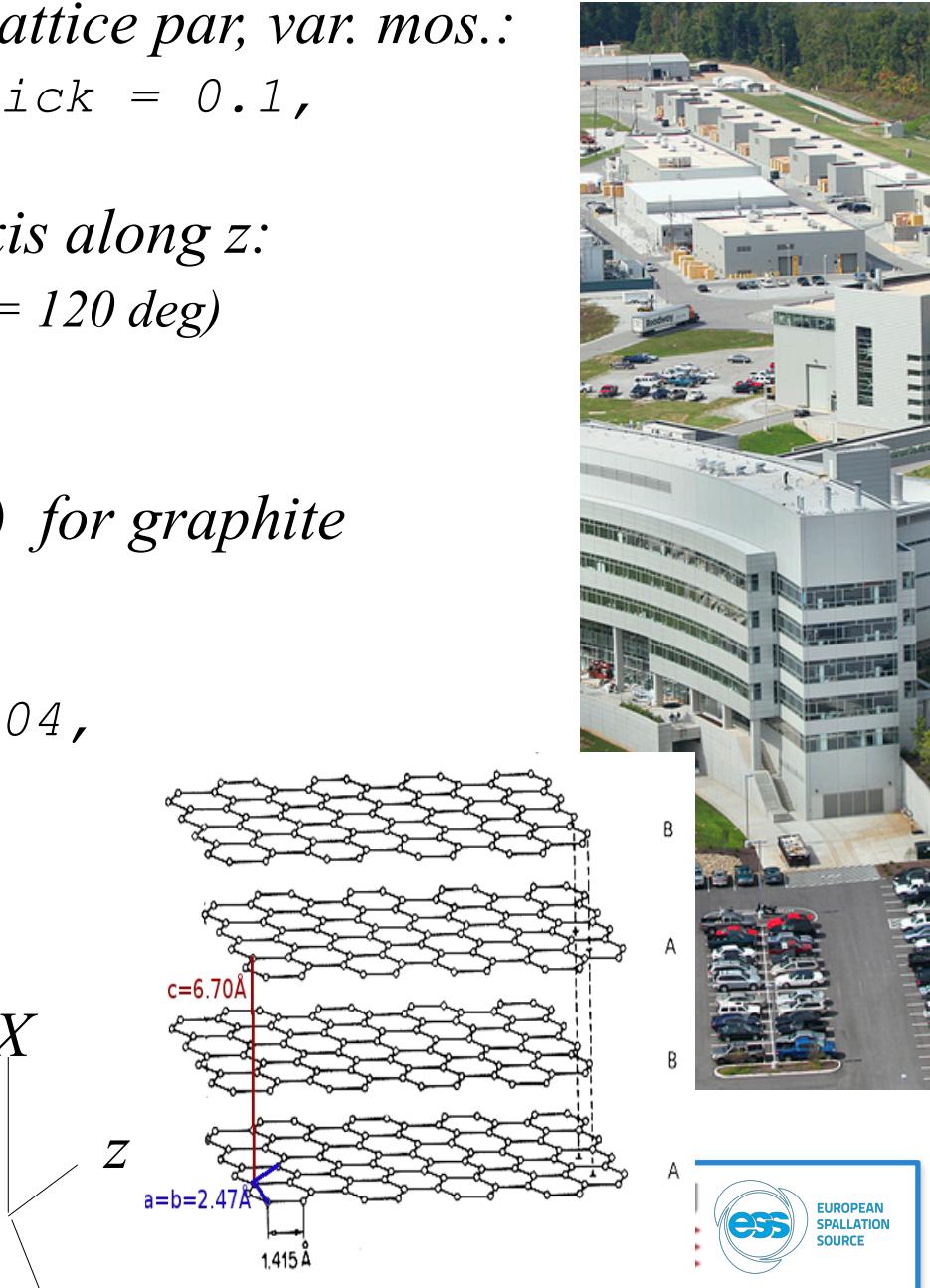
Parameters in **boldface** are required; the others are optional.

Name	Unit	Description	Default
mosaic_AB	arc_minutes, arc_minutes, 1, 1, 1, 1, 1	In Plane mosaic rotation and plane vectors (anisotropic), mosaic_A, mosaic_B, A_h,A_k,A_l, B_h,B_k,B_l. Puts the crystal in the in-plane mosaic state. Vectors A and B define plane in which the crystal roation is defined, and mosaic_A, mosaic_B, denotes the resp. mosaicities (gaussian RMS) with respect to the two reflections chosen by A and B (Miller indices).	Mosaic_AB_Undefined
reflections	string	File name containing structure factors of reflections. Use empty ("") or NULL for incoherent scattering only	0
geometry	str	Name of an Object File Format (OFF) or PLY TM file for complex geometry. The OFF/PLY file may be generated from XYZ coordinates using qhull/powercrust	0
xwidth	m	Width of crystal	0
yheight	m	Height of crystal	0
zdepth	m	Depth of crystal (no extinction simulated)	0
radius	m	Outer radius of sample in (x,z) plane	0
delta_d_d	1	Lattice spacing variance, gaussian RMS	1e-4
mosaic	arc minutes	Crystal mosaic (isotropic), gaussian RMS. Puts the crystal in the isotropic mosaic model state, thus disregarding other mosaicity parameters.	-1
mosaic_a	arc minutes	Horizontal (rotation around lattice vector a) mosaic (anisotropic), gaussian RMS. Put the crystal in the anisotropic crystal vector state. I.e. model mosaicity through rotation around the crystal lattice vectors. Has precedence over in-plane mosaic model.	-1
mosaic_b	arc minutes	Vertical (rotation around lattice vector b) mosaic (anisotropic), gaussian RMS.	-1
mosaic_c	arc minutes	Out-of-plane (Rotation around lattice vector c) mosaic (anisotropic), gaussian RMS	-1
recip_cell	1	Choice of direct/reciprocal (0/1) unit cell definition	0
barns	1	Flag to indicate if F ^2 from 'reflections' is in barns or fm^2. barns=1 for laz and isotropic constant elastic scattering (reflections=NULL), barns=0 for lau type files	0
ax	AA or AA^-1	Coordinates of first (direct/recip) unit cell vector	0
ay	-	a on y axis	0
az	-	a on z axis	0
bx	AA or AA^-1	Coordinates of second (direct/recip) unit cell vector	0
by	-	b on y axis	0
bz	-	b on z axis	0
cx	AA or AA^-1	Coordinates of third (direct/recip) unit cell vector	0
cy	-	c on y axis	0
cz	-	c on z axis	0
p_transmit	1	Monte Carlo probability for neutrons to be transmitted without any scattering. Used to improve statistics from weak reflections	-1
sigma_abs	barns	Absorption cross-section per unit cell at 2200 m/s	0
sigma_inc	barns	Incoherent scattering cross-section per unit cell Use -1 to unactivate	0
aa	deg	Unit cell angles alpha, beta and gamma. Then uses norms of vectors a,b and c as lattice parameters	0
bb	deg	Beta angle	0
cc	-	Gamma angle [deg].	0
order	1	Limit multiple scattering up to given order (0: all, 1: first, 2: second, ...)	0
RX	m	Radius of horizontal along X lattice curvature. flat for 0	0
RY	m	Radius of vertical lattice curvature. flat for 0	0
RZ	m	Radius of horizontal along Z lattice curvature. flat for 0	0
powder	1	Flag to indicate powder mode, for simulation of Debye-Scherrer cones via random crystallite orientation	0
PG	1	Flag to indicate "Pyrolytic Graphite" mode, only meaningful with choice of Graphite.lau, models PG crystal	0



Single_crystal - Basic setup

- A 2mm slab 0.1m*0.1m, small variance of lattice par, var. mos.:
 $xwidth = 0.002$, $yheight = 0.1$, $zthick = 0.1$,
 $\delta_d = 1e-4$, $mosaic = MOS$
- 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 = "C_graphite.lau",
- σ_{abs} , σ_{inc} [barns] for graphite
 $\sigma_{abs} = 0.014$, $\sigma_{inc} = 0.004$,
- Multiple scattering order = 0 (all)
- Set monochromator rotation angle α_1 in scattering condition
- Set the monitors $a2$ at the Bragg angle





Single_crystal

Play!

- Set a broader wavelength band from the source ($2.1\text{-}4.1 \text{ \AA}$)
- 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 cross-section to observe the effect
- Or with the mosaicity or variance of lattices-pacing

Single_crystal

$\lambda=4.0\text{-}4.1\text{\AA}$

$\lambda=2.1\text{-}4.1\text{\AA}$

