



Peter Willendrup

Samples in McStas - an overview



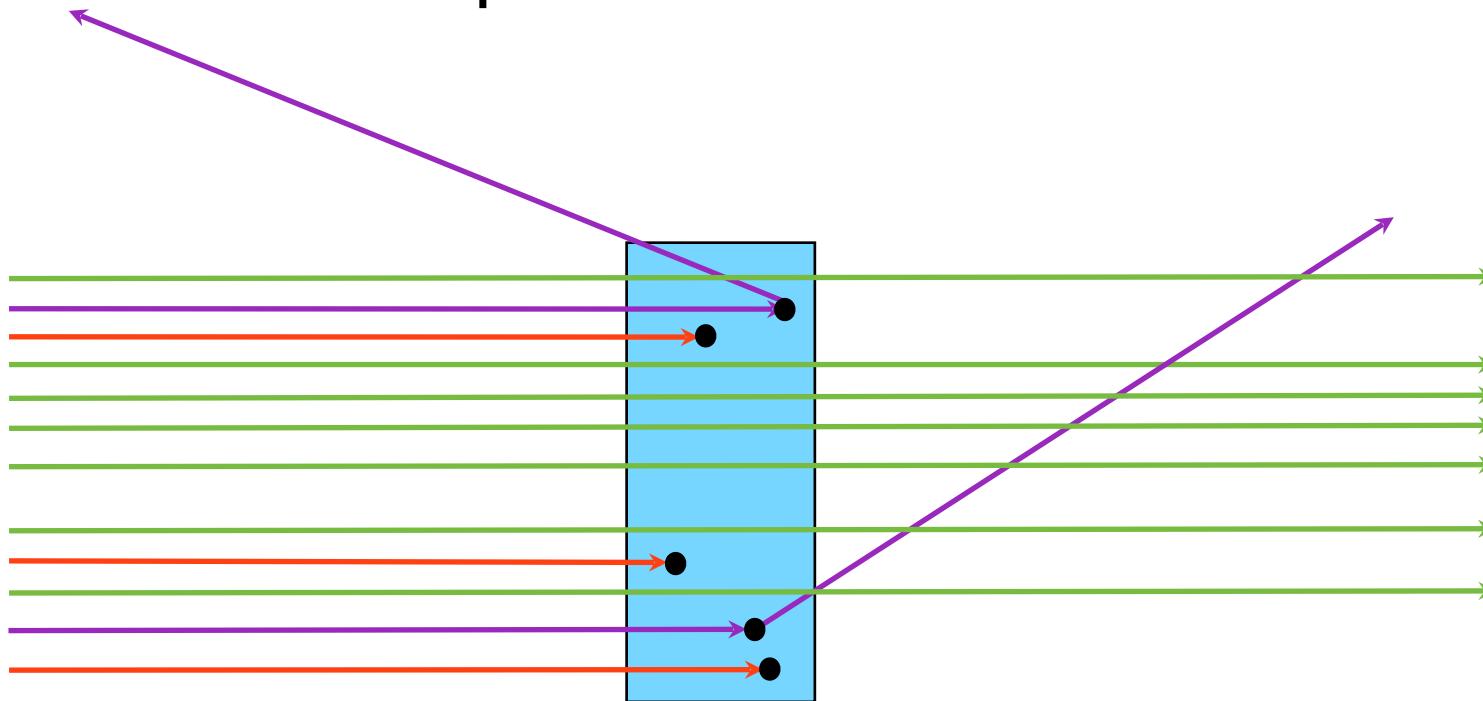
Agenda

- General concepts (reminder)
- Overview of samples in McStas
- Focus on diffraction-oriented samples:
 - Incoherent scatterer
 - Powder
 - Single Crystal
 - File formats

(Sessions on SANS and inelastic samples will follow thursday!)



Samples in General



A neutron hitting a sample can be:
absorbed, **transmitted**, or **scattered**

Samples



For a **non-thin** sample the probabilities for **absorption**, **transmission** or **scattering** are given by

$$p_A = (1 - e^{-\Sigma_T t})(\Sigma_A / \Sigma_T)$$

$$p_S = (1 - e^{-\Sigma_T t})(\Sigma_S / \Sigma_T)$$

$$p_T = 1 - p_S - p_A = e^{-\Sigma_T t}$$

t = sample thickness

$$\Sigma_* = \rho \sigma_*$$

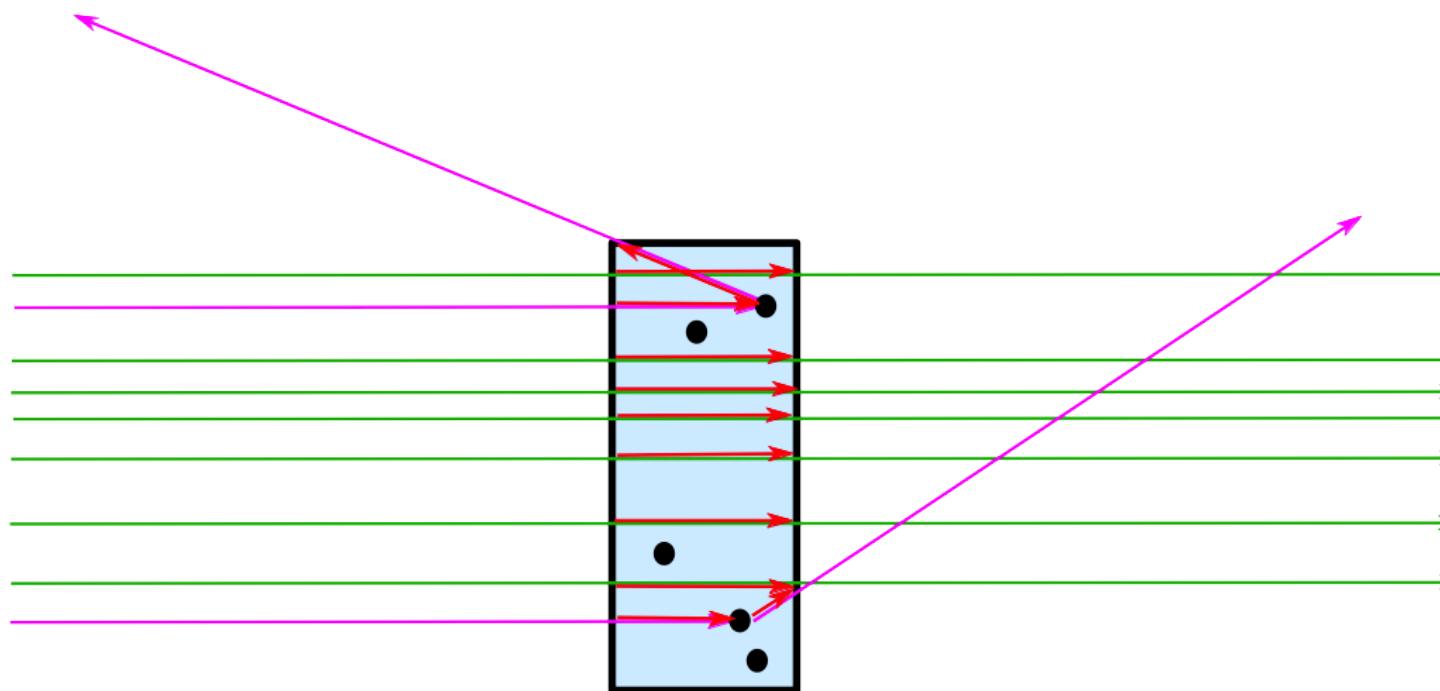


macroscopic cross section [cm⁻¹]

number density [atoms/cm³] | barn = 10⁻²⁴cm²

microscopic cross section [barn/atom]

Samples in General in McStas



A neutron ray hitting a sample can be:
transmitted+absorption, or scattered+absorption

Sample components in McStas v.2.5

 McStas  DTU	Sample Process	Coherent Elastic		Incoherent Elastic		Absorption	Multiple Scattering
		Inelastic	Inelastic	Elastic	Inelastic		
	Incoherent	No	No	Yes	No	Yes	Yes
	PowderN	Yes	No	Yes	No	Yes	Yes
	Single_crystal	Yes	No	Yes	No	Yes	Yes
	Isotropic_Sqw	Yes	Yes	Yes	Yes	Yes	Yes
	Sans_spheres	Yes	No	Yes	No	Yes	No
	SasView_models	Yes	No	Yes	No	Yes	No
	Phonon_simple	No	Yes	No	No	No	No
	Magnon_bcc	No	Yes	No	No	No	No
2021 Virtual ISIS McStas School	Single_crystal_inelastic	Yes	Yes	Yes	No	Yes	Yes

McStas sample overview table



McStas sample model functionality-matrix - McStas - ESS Confluence - Mozilla Firefox

Pages / McStas SPACE

McStas sample model functionality-matrix

Created by Peter Willendrup, last modified on Jun 19, 2018

(Master version available at the URL <https://confluence.esss.lu.se/display/MCSTAS/McStas+sample+model+functionality-matrix>)

Status of the McStas sample components, relevant for McStas 2.4.1 (Released summer 2017)

See also: [McStas sample models for Diffraction](#), [McStas sample models for Imaging](#), [McStas sample models for Large-scale Structures](#), [McStas sample models for Spectroscopy](#)

McStas sample comp + author info in italic	Model description	Main use areas	Incoherent scattering	Absorption	Bragg or other elastic scattering (type)	Inelastic scattering (type)	Multiple scattering	Non-trivial sample geometry
1 Incoherent (Vanadium, Plexiglass etc.) <i>McStas team</i>	Simple incoherent scatterer	Generic, imaging	✓	✓	✗	✗	✓	✓
2 Tunelling_sample <i>McStas team / Kim Lefmann</i>	Idem 1, plus tunneling peaks and QE broadening	Quasi-elastic scattering, backscattering	✓	✓	✗	✗ (Quasielastic broadening + tunnel peaks) (analytic approach)	(✓ analytic approach)	✓
3 PowderN <i>McStas team / Peter Willendrup</i>	Debye-scherrer cones, tabular input (lau / laz)	Powder diffraction, imaging	✓	✓	✓ (Debye-Scherrer cones)	✗	✗	✓
4 Sample_nxs <i>Mirko Bojin, HZB</i>	Debye-scherrer cones, unit-cell / atom input list	Powder diffraction, (future: imaging)	✓	✓	✓ (Debye-Scherrer cones)	✗ ✓	✓	✗
5 Single_crystal <i>McStas team</i>	Bragg spots, tabular input (lau). "Perfect imperfect" single crystal with mosaicty / lattice variation	Single crystal and MX diffraction	✓	✓	✓ (Bragg spots)	✗	✓	✓
6 Sans_spheres (and other similar) <i>McStas team and Martin Cramer Pedersen, KU</i>	Hard spheres in thin solution and other models, defined per-component...	SANS	✓	✓	✗ - SANS	✗	✗	✗
7 SANS_benchmark2 (and a few other stand-alone models) <i>Heinrich Frielinghaus, FZJ/JCNS</i>	Experimentally-benchmarked model set for SANS	SANS	✓	✓	✗ - SANS	✗	✓ up to 10 orders	✗
8 SASview_models (yet unreleased!) <i>McStas team</i>	"Any" model from SASview / SASmodels	SANS	✓	✓	✗ - SANS	✗	✗ at this point	✗

McStas sample table overview



McStas sample model functionality-matrix - Mozilla Firefox

https://confluence.esss.lu.se/display/MCSTAS/McStas+sample+model+functionality-matrix

But since it is impossible to read this table – here's where it's at:

McStas sample comp + author info in italic	Model description	Main use areas	Incoherent scattering	Absorption	Bragg or other elastic scattering (type)	Inelastic scattering (type)	Multiple scattering	Non-trivial sample geometry
<i>McStas team</i>								
9 <i>Multilayer_sample Rob Dalgleish, ISIS STFC</i>	Multilayer-sample (dynamic scattering theory) with incoherent background	Reflectometry	✓	✓	✓ - Reflectivity curve	✗	✗	✗
10 <i>Phonon_simple McStas team / Kim Lefmann</i>	Single-branch acoustic phonon in FCC lattice	Inelastic scattering phonons	✗	✗	✗	✓ (phonon, at this point FCC lattice only)	✗	✗
11 <i>Isotropic_Sqw McStas team / Emmanuel Farhi</i>	Structure and dynamics in isotropic materials (liquids, powders etc.)	Inelastic scattering, diffraction, Isotropic materials, Imaging	✓	✓	✓ (Debye-Scherrer cones)	✓ isotropic inelastic scattering	✓	✓
12 <i>Res_sample McStas team</i>	Resolution-oriented sample component	Generic	✗✓	✗	✗	*✓ flat, isotropic inelastic scattering	✗	✗
13 <i>TOFRes_sample</i>	Item Res_sample, with TOF	Generic	✗✓	✗	✗	*✓ flat, isotropic inelastic	✗	✗

available in repo available in repo available in repo not yet available in repo not yet available in repo available in repo available in repo not yet available in repo available in repo

17 "4D S(vec(Q),omega)" Duc Le - soon at ISIS STFC?	Ala Isotropic_Sqw, but with crystal lattice	Elastic and Inelastic experiments with crystals	✓	✓	✓	✓	✓	✓	? ↗?
18 "Polycrystal" Alberto Cereser + Erik Knudsen, DTU Physics	Engineering-diffraction / Imaging oriented multigrain sample	Engineering-diffraction / Imaging	✓	✓	✓ (Bragg spots)	✗	✓	✓	✓
19 "Magnetic single crystal" Linda Udby KU, + Erik Knudsen, DTU	Bragg spots from lattice ala Single_crystal plus magnetic lattice. Tabular input (lau)	Single crystal magnetic diffraction	✓	✓	✓ (Bragg spots)	✗	✓	✓	✓ / ? ↗?
20 "Reflectometry sample" Jochen Stahn, PSI	Reflectivity-curve sample	Reflectometry	✓	✓	✓ - Reflectivity curve	✗	✗	✗	✗

No labels

Incoherent Sample

McStas



[Incoherent.comp](#)

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

An incoherent scatterer with various sample shape options

Name	Unit	Description	Default
geometry	str	Name of an Object File Format (OFF) or PLY file for complex geometry. The OFF/PLY file may be generated from XYZ coordinates using qhull/powercrust	0
radius	m	Outer radius of sample in (x,z) plane	0
xwidth	m	Horiz. dimension of sample (bounding box if off file), as a width	0
yheight	m	Vert. dimension of sample (bounding box if off file), as a height. A sphere shape is used when 0 and radius is set	0
zdepth	m	Depth of sample (bounding box if off file)	0
thickness	m	Thickness of hollow sample	0
target_x	-		0
target_y	m	position of target to focus at	0
target_z	-		0
focus_r	m	Radius of disk containing target. Use 0 for full space	0
focus_xw	m	horiz. dimension of a rectangular area	0
focus_yh	m	vert. dimension of a rectangular area	0
focus_aw	deg	horiz. angular dimension of a rectangular area	0
focus_ah	deg	vert. angular dimension of a rectangular area	0
target_index	1	Relative index of component to focus at, e.g. next is +1	0
pack	1	Packing factor	1
p_interact	1	MC Probability for scattering the ray; otherwise transmit	1
f_QE	1	Fraction of quasielastic scattering (rest is elastic)	0
gamma	1	Lorentzian width of quasielastic broadening (HWHM)	0
sigma_abs	barns	Absorption cross section pr. unit cell at 2200 m/s	5.08
sigma_inc	barns	Incoherent scattering cross section pr. unit cell	5.08
Vc	AA ³	Unit cell volume	13.827
concentric	1	Indicate that this component has a hollow geometry and may contain other components. It should then be duplicated after the inside part (only for box, cylinder, sphere)	0
order	-	Limit multiple scattering up to given order	0

Incoherent Sample

McStas



[Incoherent.comp](#)

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

Name	Unit	Description	Default
geometry	str	Name of an Object File Format (OFF) or PLY file for complex geometry. The OFF/PLY file may be generated from XYZ coordinates using qhull/powercrust	0
radius	m	Outer radius of sample in (x,z) plane	0
xwidth	m	Horiz. dimension of sample (bounding box if off file), as a width	0
yheight	m	Vert. dimension of sample (bounding box if off file), as a height. A sphere shape is used when 0 and radius is set	0
zdepth	m	Depth of sample (bounding box if off file)	0
thickness	m	Thickness of hollow sample	0
target_x	-		0
target_y	m	position of target to focus at	0
target_z	-		0
focus_r	m	Radius of disk containing target. Use 0 for full space	0
focus_xw	m	horiz. dimension of a rectangular area	0
focus_yh	m	vert. dimension of a rect	
focus_aw	deg	horiz. angular dimension	
focus_ah	deg	vert. angular dimension	
target_index	1	Relative index of component	
pack	1	Packing factor	
p_interact	1	MC Probability for scatter	
I_QE	1	Fraction of quasielastic intensity	
gamma	1	Lorentzian width of quasielastic intensity	
sigma_abs	barns	Absorption cross section	
sigma_inc	barns	Incoherent scattering cross section	
Vc	AA ³	Unit cell volume	13.827
concentric	1	Indicate that this component has a hollow geometry and may contain other components. It should then be duplicated after the inside part (only for box, cylinder, sphere)	0
order	-	Limit multiple scattering up to given order	0

An incoherent scatterer with various sample shape options

p_interact = The probability that a given ray will interact (scatter) with a sample. Does not directly affect the intensity – only the quality of the resulting Monte Carlo estimate.

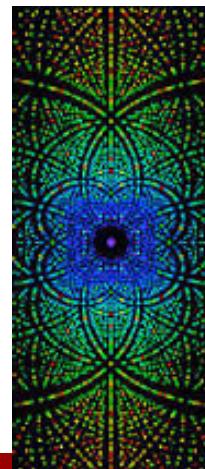


Crystalline Samples

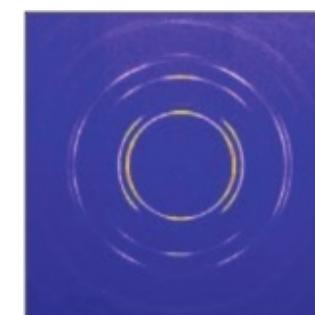
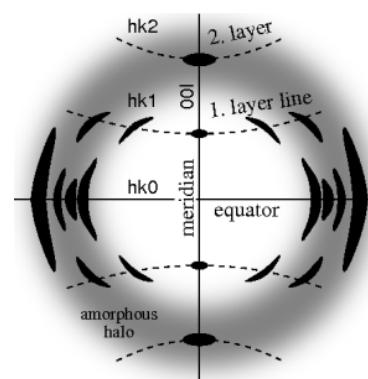




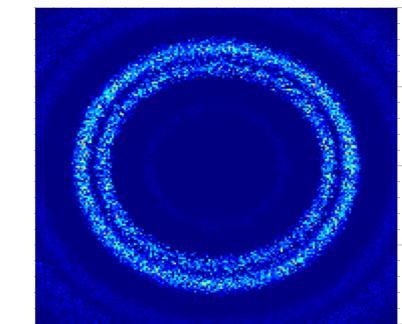
- Single crystal



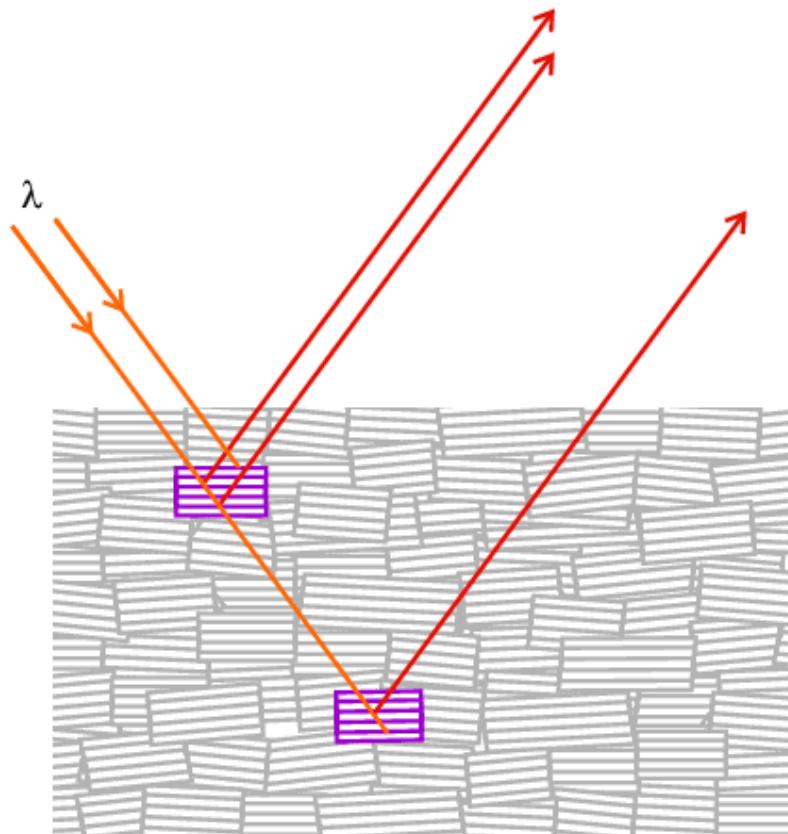
- Polycrystal with a little disorder,
i.e. a *preferred orientation, texture*



- Powder with complete disorder



Single Crystal model



- *Models ideally imperfect crystal:*
- *Peak broadening is dominated by mosaic*
=> not appropriate for highly perfect crystals.
- “Space group symmetries” considered out of scope.
 - Optimized for small unit cells but...
 - No assumption about unit cell, orientation etc.
 - Gaussian model for mosaic (see later)

Courtesy University College London

Single Crystal



McStas



DTU
EUROPEAN SPALLATION SOURCE

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 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	no extinction simulated	[m] Depth of crystal	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			0
az			0
bx	AA or AA ⁻¹	Coordinates of second (direct/recip) unit cell vector	0
by			0
bz			0
cx	AA or AA ⁻¹	Coordinates of third (direct/recip) unit cell vector	0
cy			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
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	deg	Gamma angle	0
order	0: all, 1: first, 2: second, ...	[1] Limit multiple scattering up to given order	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. A powder texture can be approximated with 0	0
PG	1	Flag to indicate "Pyrolytic Graphite" mode, only meaningful with choice of Graphite.lau, models PG crystal. A powder texture can be approximated with 0	0

Single Crystal



McStas



DTU
EUROPEAN SPALLATION SOURCE

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 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	no extinction simulated	[m] Depth of crystal	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			0
az			0
bx	AA or AA^-1	Coordinates of second (direct/recip) unit cell vector	0
by			0
bz			0
cx	AA or AA^-1		0
cy			0
cz			0
p_transm	1		-1
sigma_pos	barns		0
sigm_a_inc	barns	Incoherent scattering cross-section per unit cell Use -1 to deactivate	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	deg	Gamma angle	0
order	0: all, 1: first, 2: second, ...	[1] Limit multiple scattering up to given order	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. A powder texture can be approximated with 0	0
PG	1	Flag to indicate "Pyrolytic Graphite" mode, only meaningful with choice of Graphite.lau, models PG crystal. A powder texture can be approximated with 0	0

Unit cell vectors (ax,ay,az, bx, by,bz, cx,cy, cz). Encodes the crystal orientation relative to the Component's orientation

Single Crystal

McStas



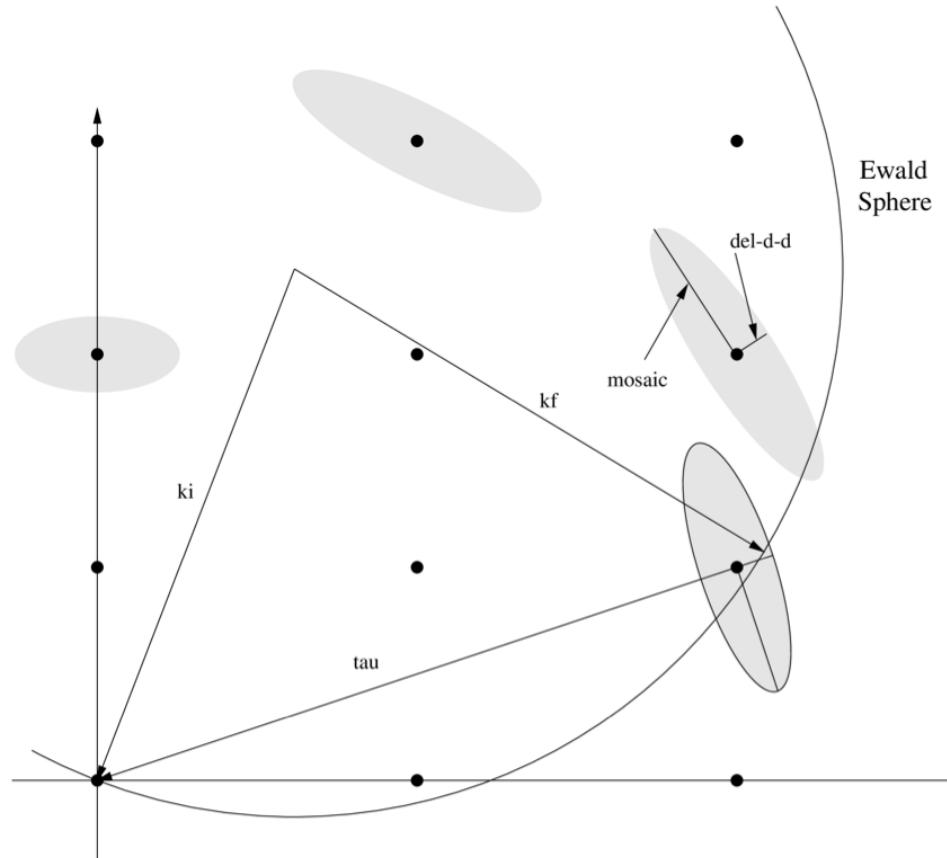
Input parameters

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

Name	Unit	Description	Default
mosaic_AB	arc_minutes, arc_minutes,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
g_mosaic	str	Name of an Object File Format (OFF) or PLY 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	no extinction simulated	[m] Depth of crystal	0
radius	m	Outer radius of sample in (x,z) plane	0
lens_d	1		1e-4
mosaic	arc minutes		-1
mosaic_a	arc minutes		-1
mosaic_b	arc minutes		-1
mosaic_c	arc minutes		-1
recip_cell	1		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			0
az			0
bx	AA or AA $^{-1}$	Coordinates of second (direct/recip) unit cell vector	0
by			0
bz			0
cx	AA or AA $^{-1}$	Coordinates of third (direct/recip) unit cell vector	0
cy			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
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	deg	Gamma angle	0
order	0, all, 1: first, 2: second, ...	[1] Limit multiple scattering up to given order	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. A powder texture can be approximated with 0	0
PG	1	Flag to indicate "Pyrolytic Graphite" mode, only meaningful with choice of Graphite.lau, models PG crystal. A powder texture can be approximated with 0	0

Mosaicity parameters: mosaic, mosaic_a, mosaic_b, mosaic_c, mosaic_AB

Single Crystal mosaicity



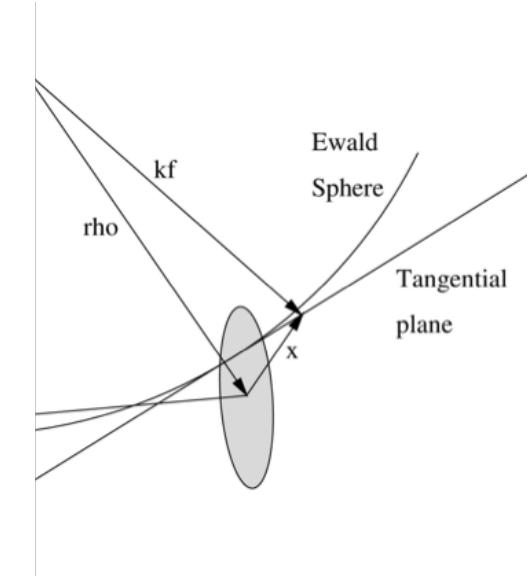
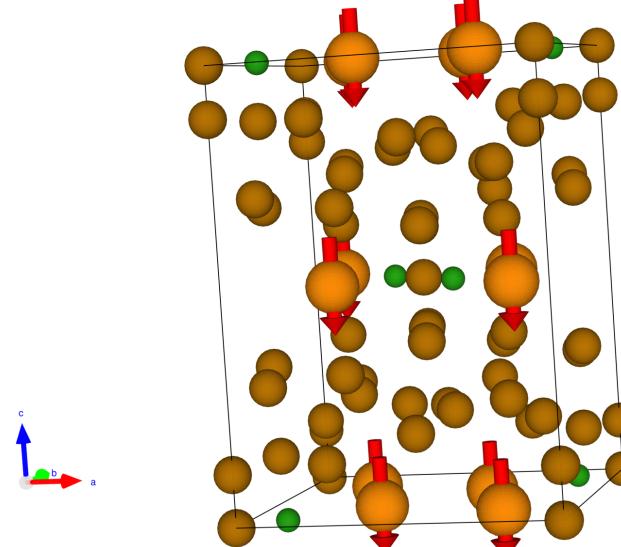


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Single Crystal mosaicity

Three models:

- Isotropic Mosaicity = Gaussian distribution of rotation angle, with given standard deviation, around a random vector.
- Anistropic mosaicity = Gaussian distribution of angles around each of the unit cell axis.

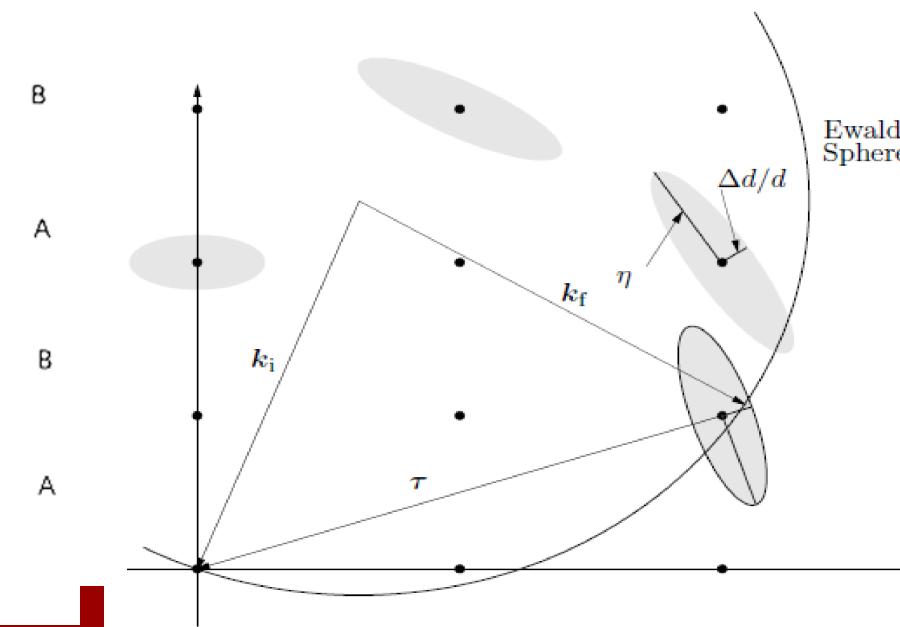
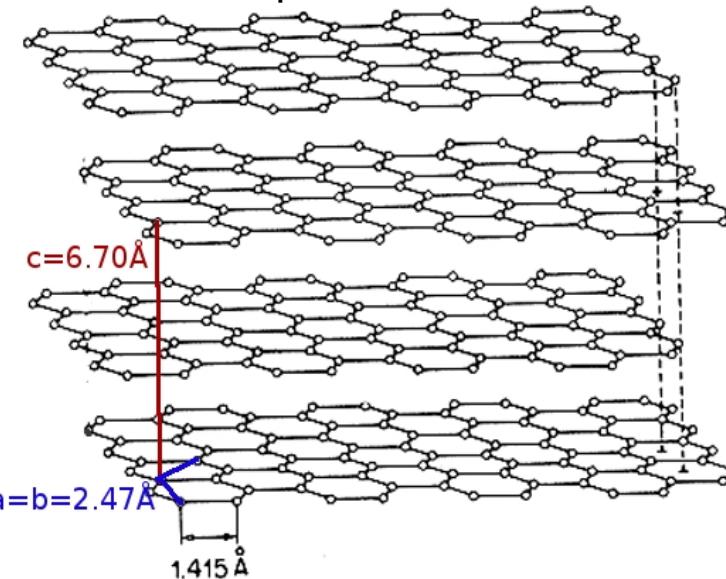


Single crystal mosaicity



Three models:

- Isotropic Mosaicity = Gaussian distribution of rotation angle, with given standard deviation, around a random vector.
- Anistropic mosaicity = Gaussian distribution of angles around each of the unit cell axis.
- “Rocking curve mosaic” = Gaussian distr. around axis determined by width of two given Bragg peaks. Specify σ , and hkl for two peaks.



9.2 PowderN



Among the most common materials measured with neutron scattering techniques are powders, which are composed of a large number of tiny single crystals. The scattering intensity, by means of constructive interference and averaging over all crystallites, appears as well defined rings around the out-going direct beam direction. These rings are also present in liquids, but are much smoother, as we shall see in next section.

Let us consider a material of density ρ made of N scattering units each with a unit cell volume V_0 arranged with lattice spacings $d_Q=2\pi/Q$ associated to structure factors $F(Q)$ with equivalent reflection multiplicities j_Q . These structure factors characterize the efficiency of the reflection with momentum exchange Q . Following Squires [14] the scattering probability for an incoming neutron with wavelength λ penetrating along a distance x into the material is about $1-\exp(-\rho\sigma_{cone}x)$ where σ_{cone} is the so-called coherent elastic cross-section of the ring,

$$\sigma_{cone} = \frac{N \pi \lambda^2 j_Q |F(Q)|^2}{V_0 Q} .$$

This relation is only valid under certain conditions, among which $d_Q > \lambda/2$, from the Bragg law. As the possible lattice spacings d in the material can not exceed a maximum value (for instance the inter-atomic distance), it appears that as the neutron wavelength increases, the number of visible rings in the diffractogram will decrease, until no more scattering is possible above the so-called *Bragg edge*, where materials become transparent to neutrons (except for absorption and incoherent scattering). This is why most of the diffractometers use thermal and hot neutrons. Cold neutrons can only scatter on large distance arrangements in materials, e.g. in larger molecules and proteins.



PowderN inputs

Input parameters

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

Name	Unit	Description	Default
format	no quotes	Name of the format, or list of column indexes (see Description).	Undefined
reflections			"NULL"
geometry	str	Name of an Object File Format (OFF) or PLY file for complex geometry. The OFF/PLY file may be generated from XYZ coordinates using qhull/powercrust	"NULL"
radius	m	Outer radius of sample in (x,z) plane	0
yheight	m	Height of sample y direction	0
xwidth	m	Horiz. dimension of sample, as a width	0
zdepth	m	Depth of box sample	0
thickness			0
pack	1	Packing factor	1
Vc	AA^3	Volume of unit cell=nb atoms per cell/density of atoms	0
sigma_abs	barns	Absorption cross section per unit cell at 2200 m/s. Use a negative value to unactivate it	0
sigma_inc	barns	Incoherent cross section per unit cell. Use a negative value to unactivate it	0
delta_d_d	0/1	Global relative delta_d_d/d broadening when the 'w' column is not available. Use 0 if ideal.	0
p_inc	1	Fraction of incoherently scattered neutron rays	0.1
p_transmit	1	Fraction of transmitted (only attenuated) neutron rays	0.1
DW	1	Global Debye-Waller factor when the 'DW' column is not available. Use 1 if included in F2	0
nb_atoms	1	Number of sub-unit per unit cell, that is ratio of sigma for chemical formula to sigma per unit cell	1
d_phi	deg	Angle corresponding to the vertical angular range to focus to, e.g. detector height. 0 for no focusing	0
p_interact	1	Fraction of events interacting with sample, e.g. 1-p_transmit-p_inc	0
concentric	only for box, cylinder, sphere	[1] Indicate that this component has a hollow geometry and may contain other components. It should then be duplicated after the inside part	0
density	g/cm^3	Density of material. rho=density/weight/1e24*N_A.	0
weight	g/mol	Atomic/molecular weight of material	0
barns	1	Flag to indicate if F ^2 from 'reflections' is in barns or fm^2 (barns=1 for laz, barns=0 for lau type files).	1
Strain	ppm	Global relative delta_d_d/d shift when the 'Strain' column is not available. Use 0 if ideal.	0
focus_flip	1	Controls the sense of d_phi. If 0 d_phi is measured against the xz-plane. If !=0 d_phi is measured against zy-plane.	0

PowderN inputs

McStas

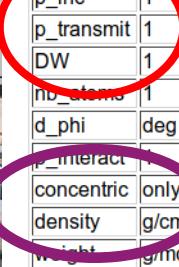


Input parameters

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

Name	Unit	Description	Default
format	no quotes	Name of the format, or list of column indexes (see Description).	Undefined
reflections			"NULL"
geometry	str	Name of an Object File Format (OFF) or PLY file for complex geometry. The OFF/PLY file may be generated from XYZ coordinates using qhull/powercrust	"NULL"
radius	m	Outer radius of sample in (x,z) plane	0
yheight	m	Height of sample y direction	0
xwidth	m	Horiz. dimension of sample, as a width	0
zdepth	m	Depth of box sample	0
thickness			0
pack	1	Packing factor	1
Vc	AA^3	Volume of unit cell=nb atoms per cell/density of atoms	0
sigma_abs	barns	Absorption cross section per unit cell at 2200 m/s. Use a negative value to unactivate it	0
sigma_inc	barns	Incoherent cross section per unit cell. Use a negative value to unactivate it	0
delta_d_d	0/1	In the 'w' column is not available. Use 0 if ideal.	0
p_inc	1	Fraction of transmitted (only attenuated) neutron rays	0.1
p_transmit	1		0.1
DW	1	Global Debye-Waller factor when the 'DW' column is not available. Use 1 if included in F2	0
nb_subunits	1	Number of sub-unit per unit cell, that is ratio of sigma for chemical formula to sigma per unit cell	1
d_phi	deg	Angle corresponding to the vertical angular range to focus to, e.g. detector height. 0 for no focusing	0
p_interact	1	Fraction of events interacting with sample, e.g. 1-p_transmit-p_inc	0
concentric	only for box, cylinder, sphere	[1] Indicate that this component has a hollow geometry and may contain other components. It should then be duplicated after the inside part	0
density	g/cm^3	Density of material. rho=density/weight/1e24*N_A.	0
weight	g/mol	Atomic/molecular weight of material	0
barns	1	Flag to indicate if F ^2 from 'reflections' is in barns or fm^2 (barns=1 for laz, barns=0 for lau type files).	1
Strain	ppm	Global relative delta_d_d shift when the 'Strain' column is not available. Use 0 if ideal.	0
focus_flip	1	Controls the sense of d_phi. If 0 d_phi is measured against the xz-plane. If !=0 d_phi is measured against zy-plane.	0

Sampling parameters



Concentric = Hollow
Powder [cylinder]



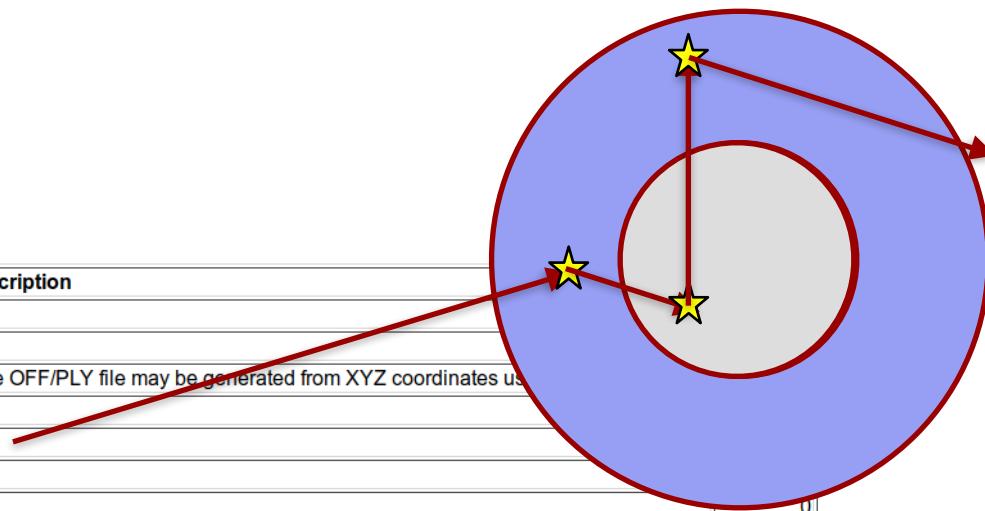
PowderN inputs

Input parameters

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

Name	Unit	Description
format	no quotes	Name of the format, or list of column indexes (see Description).
reflections		
geometry	str	Name of an Object File Format (OFF) or PLY file for complex geometry. The OFF/PLY file may be generated from XYZ coordinates us
radius	m	Outer radius of sample in (x,z) plane
yheight	m	Height of sample y direction
xwidth	m	Horiz. dimension of sample, as a width
zdepth	m	Depth of box sample
thickness		
pack	1	Packing factor
Vc	AA^3	Volume of unit cell=nb atoms per cell/density of atoms
sigma_abs	barns	Absorption cross section per unit cell at 2200 m/s. Use a negative value to unactivate it
sigma_inc	barns	Incoherent cross section per unit cell. Use a negative value to unactivate it
delta_d_d	0/1	In the 'w' column is not available. Use 0 if ideal.
p_inc	1	
p_transmit	1	Fraction of transmitted (only attenuated) neutron rays
DW	1	Global Debye-Waller factor when the 'DW' column is not available. Use 1 if included in F2
nb_subunits	1	Number of sub-unit per unit cell, that is ratio of sigma for chemical formula to sigma per unit cell
d_phi	deg	Angle corresponding to the vertical angular range to focus to, e.g. detector height. 0 for no focusing
p_interact	1	Fraction of events interacting with sample, e.g. 1-p_transmit-p_inc
concentric	only for box, cylinder, sphere	[1] Indicate that this component has a hollow geometry and may contain other components. It should then be duplicated after the inside part
density	g/cm^3	Density of material. rho=density/weight/1e24*N_A.
weight	g/mol	Atomic/molecular weight of material
barns	1	Flag to indicate if F ^2 from 'reflections' is in barns or fm^2 (barns=1 for laz, barns=0 for lau type files).
Strain	ppm	Global relative delta_d_d shift when the 'Strain' column is not available. Use 0 if ideal.
focus_flip	1	Controls the sense of d_phi. If 0 d_phi is measured against the xz-plane. If !=0 d_phi is measured against zy-plane.

Sampling parameters



Concentric = Hollow
Powder [cylinder]

Powder

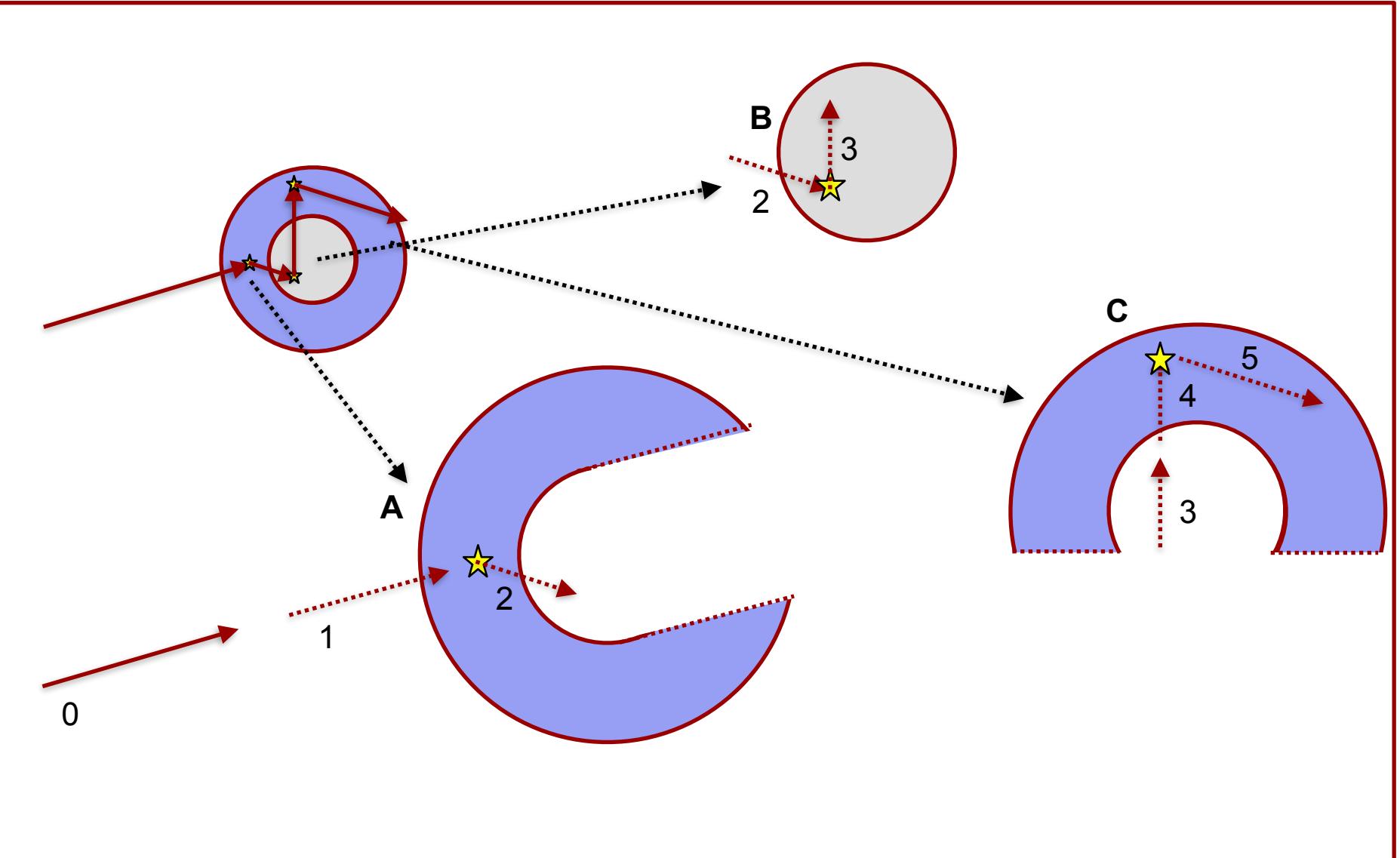


McStas

Input parameters

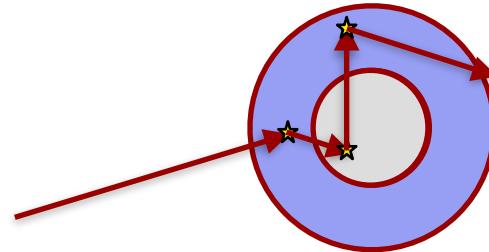
Parameters in **boldface** are re

Name	Unit
format	no quotes
reflections	
geometry	str
radius	m
yheight	m
xwidth	m
zdepth	m
thickness	
pack	1
Vc	AA^3
sigma_abs	barns
sigma_inc	barns
delta_d_d	0/1
p_inc	1
p_transmit	1
DW	1
nb_scans	1
d_phi	deg
p_interact	
concentric	only for box, cylinder
density	g/cm^3
weight	g/mol
barns	1
Strain	ppm
focus_flip	1



Concentric = Hollow
Powder [cylinder]

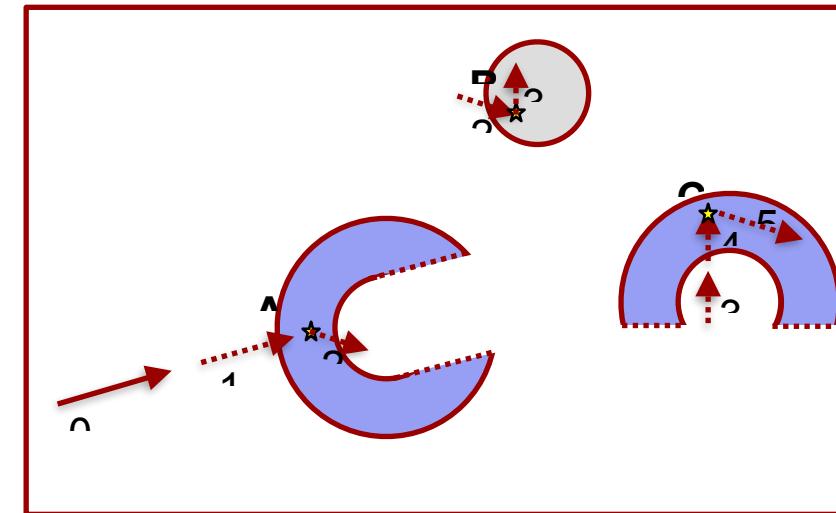
PowderN concentric in code



```
COMPONENT Al = PowderN(
    reflections="Al.laz", radius=0.02, yheight=0.05, thickness=0.005,
    p_transmit=0.8, concentric=1)
AT (0, 0, 0) RELATIVE PREVIOUS
```

```
COMPONENT a12co3 = PowderN(
    reflections=Al2CO3-laz, radius=0.005, yheight=0.05,
    p_inc=0.15, p_transmit=0.5)
AT (0, 0, 0) RELATIVE PREVIOUS
```

```
COMPONENT Al_2 = COPY(Al) (concentric=0)
AT (0,0,0) RELATIVE PREVIOUS
```



PowderN inputs

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ISIS
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Input parameters

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

Name	Unit	Description	Default
format	no quotes	Name of the format, or list of column indexes (see Description).	Undefined
reflections			"NULL"
geometry	str	Name of an Object File Format (OFF) or PLY file for complex geometry. The OFF/PLY file may be generated from XYZ coordinates using qhull/powercrust	"NULL"
radius	m	Outer radius of sample in (x,z) plane	0
yheight	m	Height of sample y direction	0
xwidth	m	Horiz. dimension of sample, as a width	0
zdepth	m	Depth of box sample	0
thickness			0
pack	1	Packing factor	1
Vc	AA^3	Volume of unit cell=nb atoms per cell/density of atoms	0
sigma_abs	barns	Absorption cross section per unit cell at 2200 m/s. Use a negative value to unactivate it	0
sigma_inc	barns	Incoherent cross section per unit cell. Use a negative value to unactivate it	0
delta_d_d	0/1	Global relative delta_d_d/d broadening when the 'w' column is not available. Use 0 if ideal.	0
p_inc	1	Fraction of incoherently scattered neutron rays	0.1
p_transmit	1	Fraction of transmitted (only attenuated) neutron rays	0.1
DW	1	Global Debye-Waller factor when the 'DW' column is not available. Use 1 if included in F2	0
nb_atoms	1	Number of sub-unit per unit cell, that is ratio of sigma for chemical formula to sigma per unit cell	1
d_phi	deg	Angle corresponding to the vertical angular range to focus to, e.g. detector height. 0 for no focusing	0
p_interact	1	Fraction of events interacting with sample, e.g. 1-p_transmit-p_inc	0
concentric	only for box, cylinder, sphere	[1] Indicate that this component has a hollow geometry and may contain other components. It should then be duplicated after the inside part	0
density	g/cm^3	Density of material. rho=density/weight/1e24*N_A.	0
weight	g/mol		0
barns	1	s or fm^2 (barns=1 for laz, barns=0 for lau type files).	1
Strain	ppm	column is not available. Use 0 if ideal.	0
focus_flip	1	d against the xz-plane. If !=0 d_phi is measured against zy-plane.	0

Only scatter into a part of
 4π

PowderN inputs

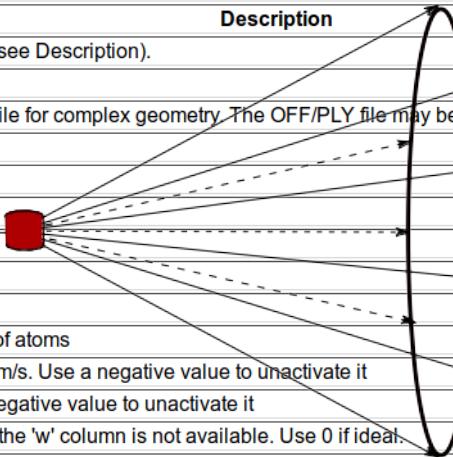
McStas
 DTU
 INSTITUTE OF
 APPLIED PHYSICS
 ESS
 EUROPEAN SPALLATION SOURCE


Input parameters

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

Name	Unit	Description	Default
format	no quotes	Name of the format, or list of column indexes (see Description).	Undefined
reflections			"NULL"
geometry	str	Name of an Object File Format (OFF) or PLY file for complex geometry. The OFF/PLY file may be generated from XYZ coordinates using qhull/powercrust	"NULL"
radius	m	Outer radius of sample in (x,z) plane	0
yheight	m	Height of sample y direction	0
xwidth	m	Horiz. dimension of sample, as a width	0
zdepth	m	Depth of box sample	0
thickness			0
pack	1	Packing factor	1
Vc	AA^3	Volume of unit cell=nb atoms per cell/density of atoms	0
sigma_abs	barns	Absorption cross section per unit cell at 2200 m/s. Use a negative value to unactivate it	0
sigma_inc	barns	Incoherent cross section per unit cell. Use a negative value to unactivate it	0
delta_d_d	0/1	Global relative delta_d_d/d broadening when the 'w' column is not available. Use 0 if ideal.	0
p_inc	1	Fraction of incoherently scattered neutron rays	0.1
p_transmit	1	Fraction of transmitted (only attenuated) neutron rays	0.1
DW	1	Global Debye-Waller factor when the 'DW' column is not available. Use 1 if included in F2	0
nb_atoms	1	Number of sub-unit per unit cell, that is ratio of sigma for chemical formula to sigma per unit cell	1
d_phi	deg	Angle corresponding to the vertical angular range to focus to, e.g. detector height. 0 for no focusing	0
p_interact	1	Fraction of events interacting with sample, e.g. 1-p_transmit-p_inc	0
concentric	only for box, cylinder, sphere	[1] Indicate that this component has a hollow geometry and may contain other components. It should then be duplicated after the inside part	0
density	g/cm^3	Density of material. rho=density/weight/1e24*N_A.	0
weight	g/mol		0
barns	1	s or fm^2 (barns=1 for laz, barns=0 for lau type files).	1
Strain	ppm	column is not available. Use 0 if ideal.	0
focus_flip	1	d against the xz-plane. If !=0 d_phi is measured against zy-plane.	0

Only scatter into a part of
 4π



PowderN inputs

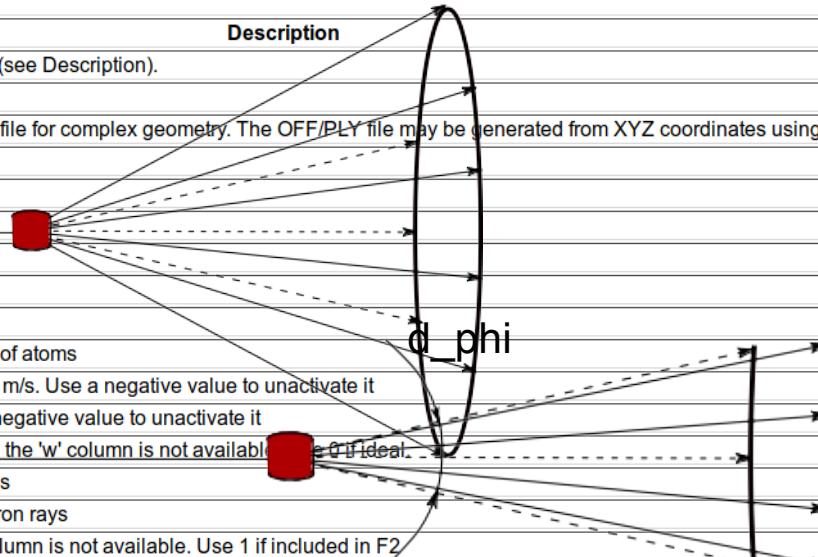


Input parameters

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

Name	Unit	Description	Default
format	no quotes	Name of the format, or list of column indexes (see Description).	Undefined
reflections			"NULL"
geometry	str	Name of an Object File Format (OFF) or PLY file for complex geometry. The OFF/PLY file may be generated from XYZ coordinates using qhull/powercrust	"NULL"
radius	m	Outer radius of sample in (x,z) plane	0
yheight	m	Height of sample y direction	0
xwidth	m	Horiz. dimension of sample, as a width	0
zdepth	m	Depth of box sample	0
thickness			0
pack	1	Packing factor	1
Vc	AA^3	Volume of unit cell=nb atoms per cell/density of atoms	0
sigma_abs	barns	Absorption cross section per unit cell at 2200 m/s. Use a negative value to unactivate it	0
sigma_inc	barns	Incoherent cross section per unit cell. Use a negative value to unactivate it	0
delta_d_d	0/1	Global relative delta_d_d/d broadening when the 'w' column is not available. Use 0 if ideal.	0
p_inc	1	Fraction of incoherently scattered neutron rays	0.1
p_transmit	1	Fraction of transmitted (only attenuated) neutron rays	0.1
DW	1	Global Debye-Waller factor when the 'DW' column is not available. Use 1 if included in F2	0
nb_atoms	1	Number of sub-unit per unit cell, that is ratio of sigma for chemical formula to sigma per unit cell	1
d_phi	deg	Angle corresponding to the vertical angular range to focus to, e.g. detector height. 0 for no focusing	0
p_interact	1	Fraction of events interacting with sample, e.g. 1-p_transmit-p_inc	0
concentric	only for box, cylinder, sphere	[1] Indicate that this component has a hollow geometry and may contain other components. It should then be duplicated after the inside part	0
density	g/cm^3	Density of material. rho=density/weight/1e24*N_A.	0
weight	g/mol		0
barns	1	s or fm^2 (barns=1 for laz, barns=0 for lau type files).	1
Strain	ppm	column is not available. Use 0 if ideal.	0
focus_flip	1	d against the xz-plane. If !=0 d_phi is measured against zy-plane.	0

Only scatter into a part of
 4π





```
# CELL 4.049320 4.049320 4.049320 90.000000 90.000000 90.000000
# SPCGRP F M 3 M CUBIC STRUCTURE
# ATOM AL 1 0.000000 0.000000 0.000000
# SCATTERING FACTOR COEFFICIENTS: AL F= 0.345 CM-12
# Reference: Physical Review (1940) 57, 198-206
#
# Physical parameters:
# sigma_coh 1.495 coherent scattering cross section (single atom) in [barn]
# sigma_inc 0.0082 incoherent scattering cross section (single atom)in [barn]
# sigma_abs 0.231 absorption scattering cross section (single atom) in [barn]
# density 2.70 in [g/cm^3]
# weight 26.98 in [g/mol] (single atom)
# multiplicity 4 in [atoms/unit cell]
# Vc 66.4 volume of unit cell in [A^3]
# v_sound 5100 in [m/s]
# v_sound_l 6420 velocity of longitudinal sound in [m/s]
# v_sound_t 3040 velocity of transversal sound in [m/s]
# T_m 933.5 melting temperature in [K]
# T_b 2792.2 boiling temperature in [K]
# At_number 13 atomic number Z
# lattice_a 4.04932 lattice parameter a in [Angs]
#
# Format parameters: Crystallographica format
# column_j 4 multiplicity 'j'
# column_d 5 d-spacing 'd' in [Angs]
```

Lau datafiles header

+

reflection list

Can be used with
Single_crystal, PowderN,
Isotropic_Sqw

Input for the PowderN



```
# TITLE *Corundum-Al2O3-[R3-CH] Graafsma, H.;Souhassou, M.;Harkem[1998] [corundum saphire:blue, ruby:red]
# CELL 4.757000 4.757000 12.987700 90.000000 90.000000 120.000000
# SPCGRP R -3 C TRIGONAL STRUCTURE
# ATOM AL 1 0.000000 0.000000 0.352110
# ATOM O 1 0.306260 0.306260 0.250000
# SCATTERING FACTOR COEFFICIENTS: AL F= 0.345 CM-12 ; O F= 0.581 CM-12
# Reference: Acta Crystallographica B (1998) 54, 193-195
#
# Physical parameters:
# sigma_coh 15.683 coherent scattering cross section for Al2O3 in [barn]
# sigma_inc 0.0188 incoherent scattering cross section for Al2O3 in [barn]
# sigma_abs 0.4625 absorption scattering cross section for Al2O3 in [barn]
# density 4.05 in [g/cm^3]
# weight 101.96 in [g/mol] for Al2O3
# multiplicity 6 in [Al2O3/unit cell]
# Vc 254.52 volume of unit cell in [A^3]
# T_m 2273 melting temperature in [K]
# T_b 3773 boiling temperature in [K]
# lattice_a 4.757 lattice parameter a in [Angs]
# lattice_c 12.9877 lattice parameter c in [Angs]
# lattice_cc 120 lattice angle gamma in [deg]
#
# Format parameters: Lazy format <http://icsd.ill.fr>
# column_j 17 multiplicity 'j'
# column_d 6 d-spacing 'd' in [Angs]
# column_F 13 norm of scattering factor |F| in [barn]
# column_h 1
```

Laz + Lau datafiles

header

+

reflection list

Can be used with PowderN,
Isotropic_Sqw

What's already there?

Single Crystals

Al.lau
 Al203_sapphire.lau
 B4C.lau
 BCC_fake.lau
 BeO.lau
 C60.lau
 C_diamond.lau
 C_graphite.lau
 CaF2.lau
 Ge.lau
 In.lau
 PPase_D_P1.lau
 Rubredoxin.lau
 Si02_cristobalite.lau
 Si02_quartz.a.lau
 Si02_quartzb.lau
 Ti02_rutile.lau
 YBaCu0.lau
 adrenaline.lau
 aspirin.lau
 leucine.lau

Powders

Ag.laz
 Al.laz
 Al203_sapphire.laz
 Au.laz
 B4C.laz
 Ba.laz
 Be.laz
 BeO.laz
 Bi.laz
 C_diamond.laz
 C_graphite.laz
 Cd.laz
 Cr.laz
 Cs.laz
 Cu.laz
 Cu2MnAl.laz
 Fe.laz
 Fe_Gamma.laz
 Ga.laz
 Gd.laz
 Ge.laz
 H2O_ice_1h.laz
 He4_hcp.laz
 Hg.laz
 I2.laz
 K.laz
 Li.laz
 LiF.laz
 Mo.laz
 Na2Ca3Al2F14.laz
 Nb.laz
 Ni.laz
 Pb.laz
 Pd.laz
 Pt.laz
 Rb.laz
 Se_alpha.laz
 Se_beta.laz
 Si.laz
 Si02_quartz.a.laz
 Si02_quartzb.laz
 Sn_alpha.laz
 Sn_beta.laz
 Ti.laz
 Tl.laz
 U02.laz
 V.laz
 Y203.laz
 Y3Fe5O12_YIG.laz
 Zn.laz
 Zr.laz
 duplex.laz

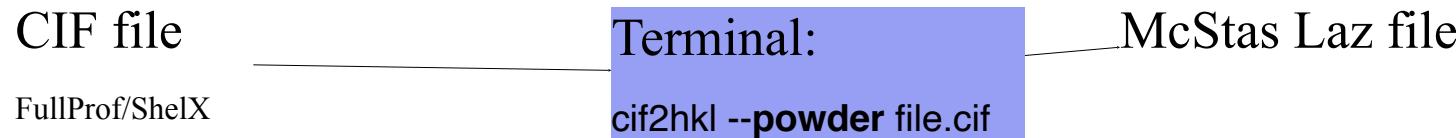
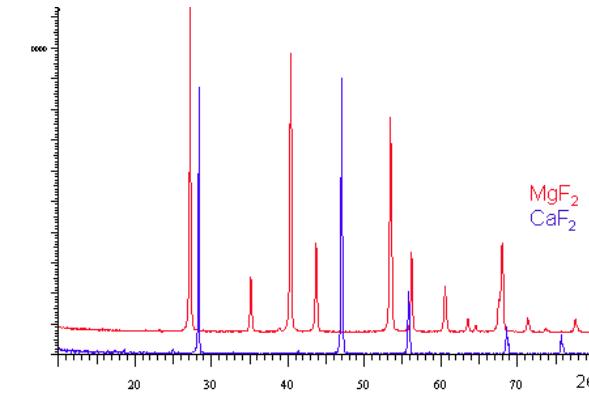
Where to get these files...



- | \$MCSTAS/data
 - | Windows: c:\mcstas-2.5\lib\data
 - | Linux: /usr/(local)/share/mcstas/2.5/data
 - | OS X: /Applications/McStas-2.5/Contents/Resources/mcstas/2.5/data
- | - Or make your own via
 - | Finding a CIF file for the given structure
 - | e.g. from
ICSD <http://icsd.fiz-karlsruhe.de> or
COD <<http://crystallography.net>>
 - | [Build one using VESTA](#)
 - | Process it using
 - | cif2hkl which is available in your McStas installation

McStas: structure: powder

- For powders, the pure elastic diffraction is easy to prepare: LAZ
 - PowderN
 - Single_crystal(powder=1, ...)
 - Isotropic_Sqw



McStas: structure: SX

- For single crystals, the pure elastic diffraction is easy to prepare: LAU
 - PowderN
 - Single_crystal
 - Isotropic_Sqw



CIF file

FullProf/ShelX

Terminal:

```
cif2hkl --xtal file.cif
```

McStas Lau file

McStas Data formats

McStas uses a number of input data formats, all text based.

- **Lau** (Single_crystal, PowderN, Isotropic_Sqw)
- **Laz** (PowderN, Isotropic_Sqw)
- **Sqw** (Isotropic_Sqw)
- **qSq** (Isotropic_Sqw) – mostly for liquids
- **nxs** (Sample_nxs) – this is *not* a NeXus/HDF
- **PDB** (SANS_PDB)
- **ncmat** (NCrystal)



OFF/PLY any geometry

An additional complex geometry enables to use any point set to describe the material volume (geomview OFF file).

