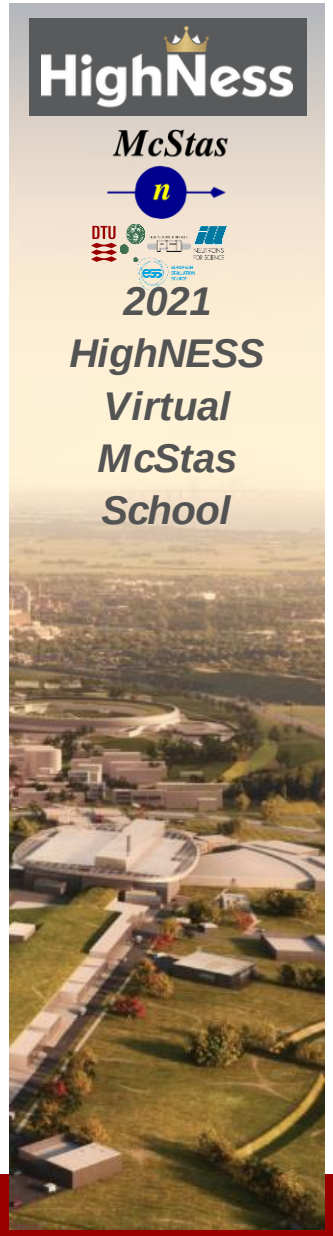
HighNESS is funded by the European Framework for Research and Innovation Horizon 2020, under grant agreement 951782

Erik Knudsen

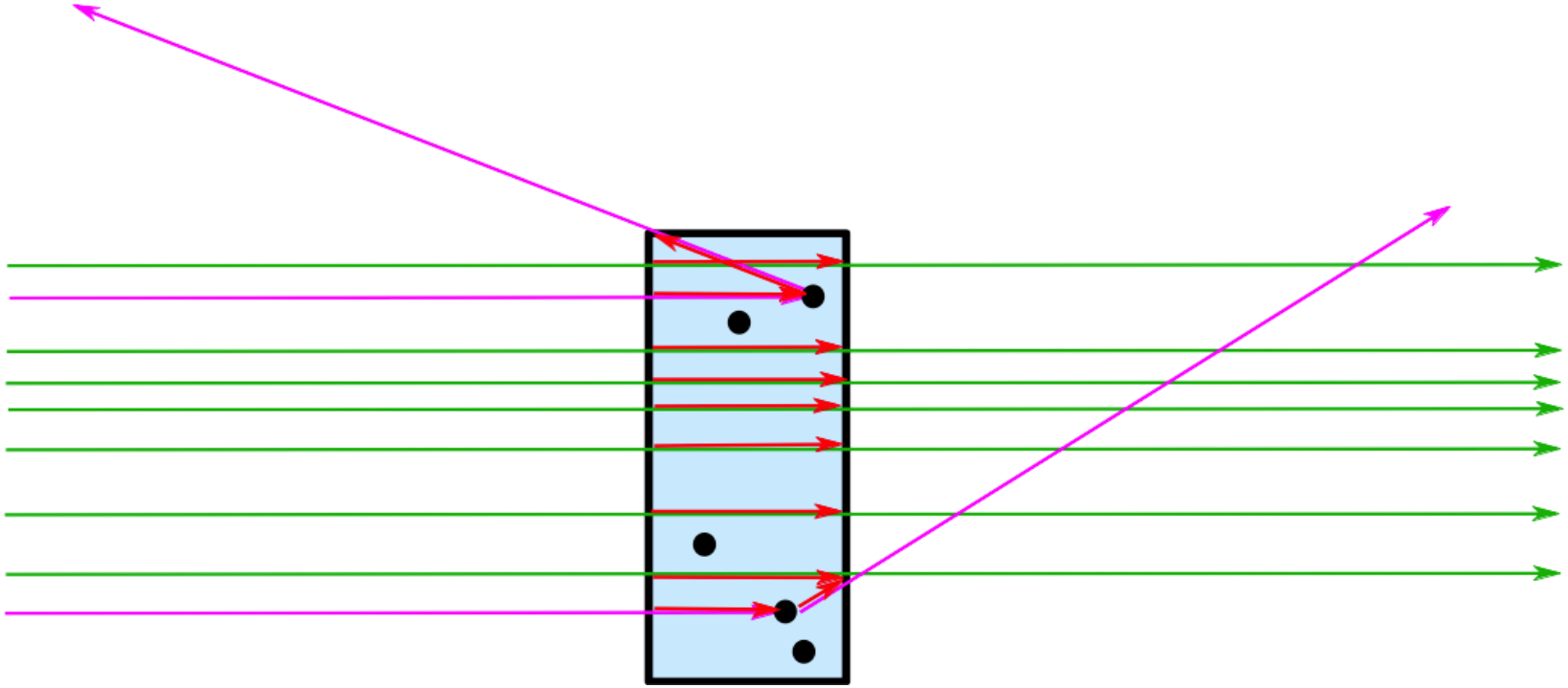
McStas samples for diffraction

Agenda

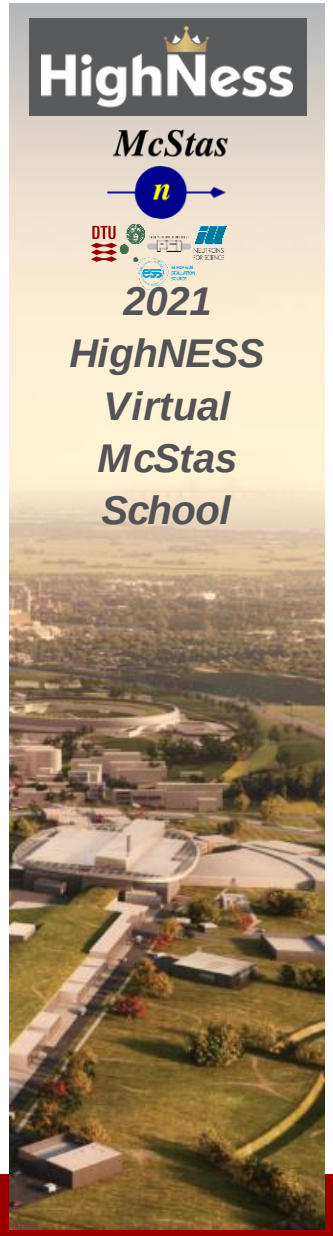


- General concepts (reminder)
- Focus on diffraction-oriented samples:
  - Incoherent scatterer
  - Powder
  - Single Crystal
  - File formats

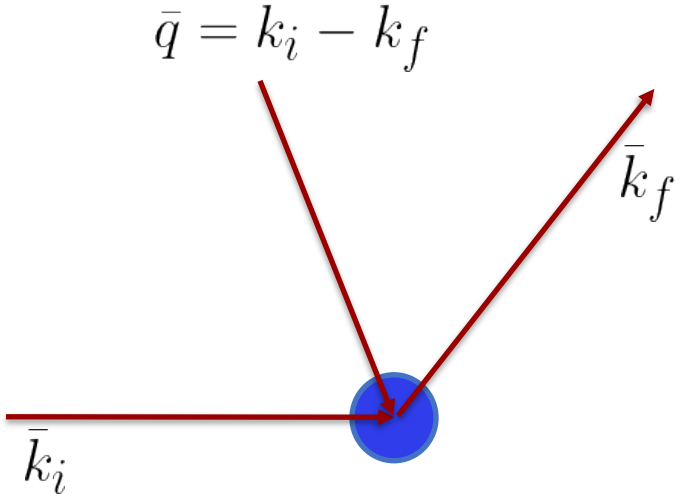
Scattering in McStas - reminder



transmitted+absorption, or scattered+absorption



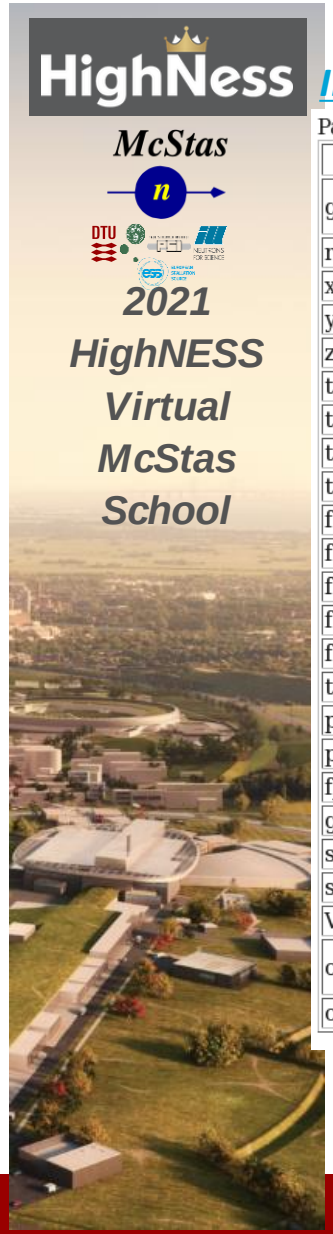
Elastic Scattering – reminder



Elastic condition:

$$\left|\bar{k}_i\right| = \left|\bar{k}_f\right|$$

Incoherent Sample



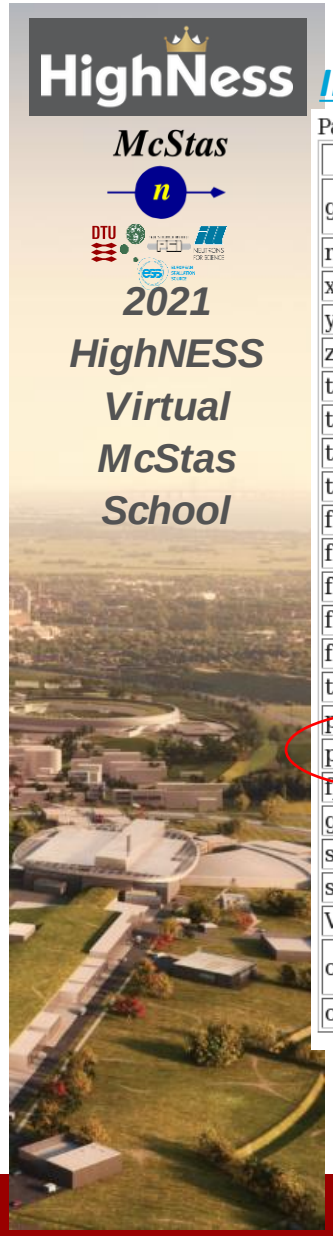
Incoherent.comp

An incoherent scatterer with various sample shape options

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 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



Incoherent.comp

An incoherent scatterer with various sample shape options

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 re	
focus_aw	deg	horiz. angular dimensi	
focus_ah	deg	vert. angular dimensio	
target_index	1	Relative index of comp	
pack	1	Packing factor	
p_interact	1	MC Probability for scat	
f_QE	1	Fraction of quasielasti	
gamma	1	Lorentzian width of qu	
sigma_abs	barns	Absorption cross secti	
sigma_inc	barns	Incoherent scattering c	
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

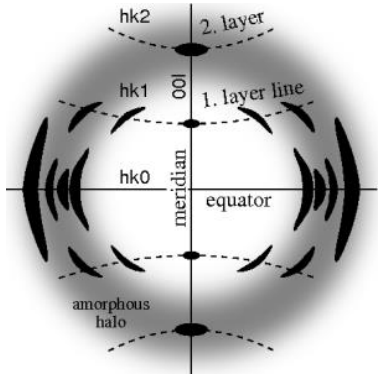
p_interact = The probability that a given ray will interact (scatter) with a sample. Does not directly affect the intensity – only the quality of the resulting Monte Carlo estimate.

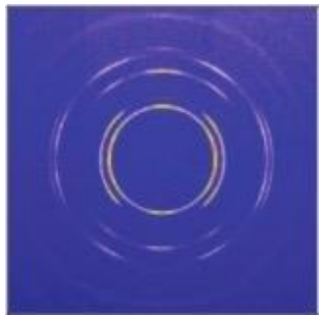
Crystalline samples

From single crystal / crystallites to powder….

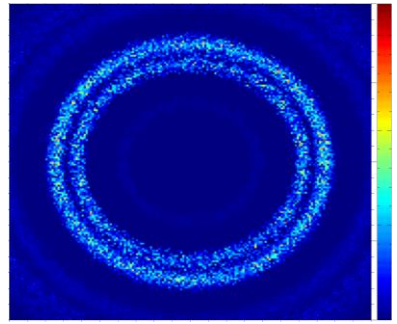
- Single crystal

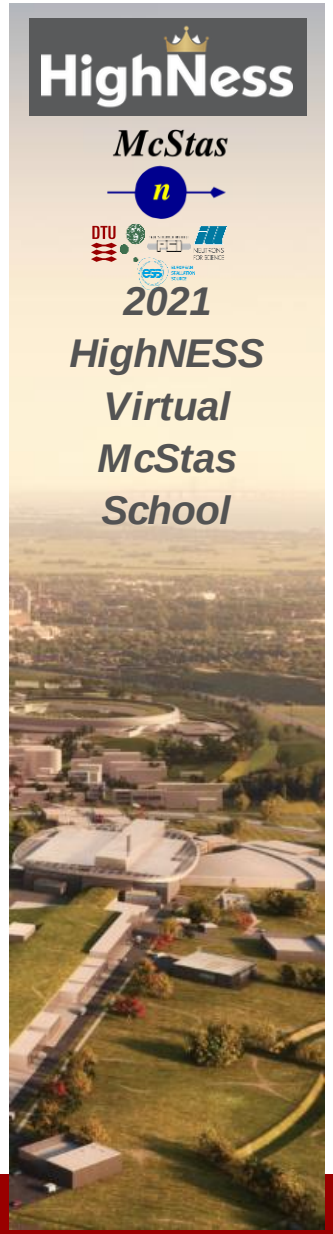
- Polycrystal with a little disorder, i.e. a *preferred orientation, texture*

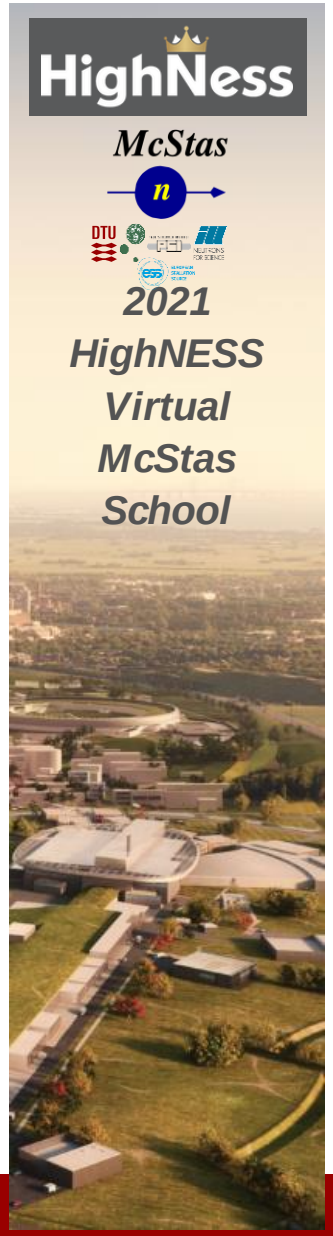




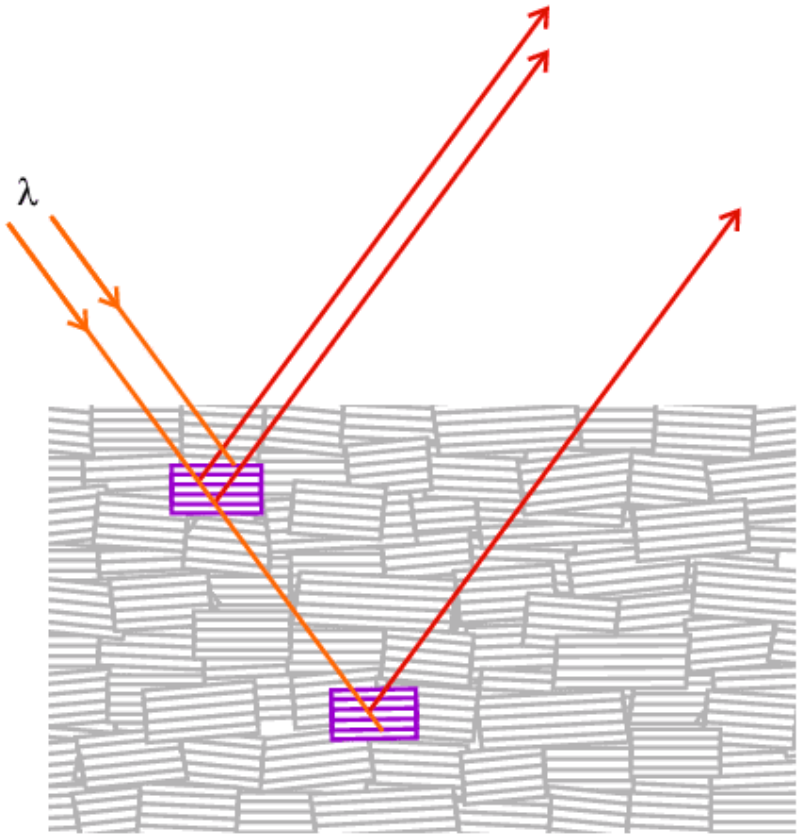
- Powder with complete disorder





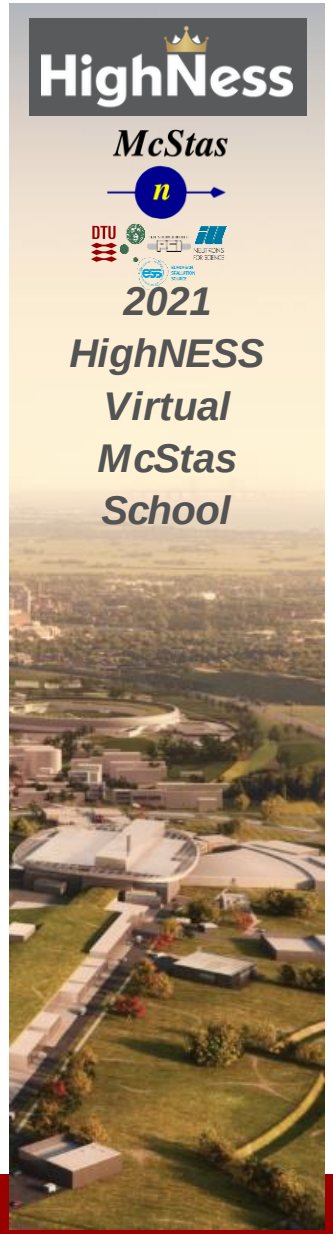


Single Crystal model



- *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

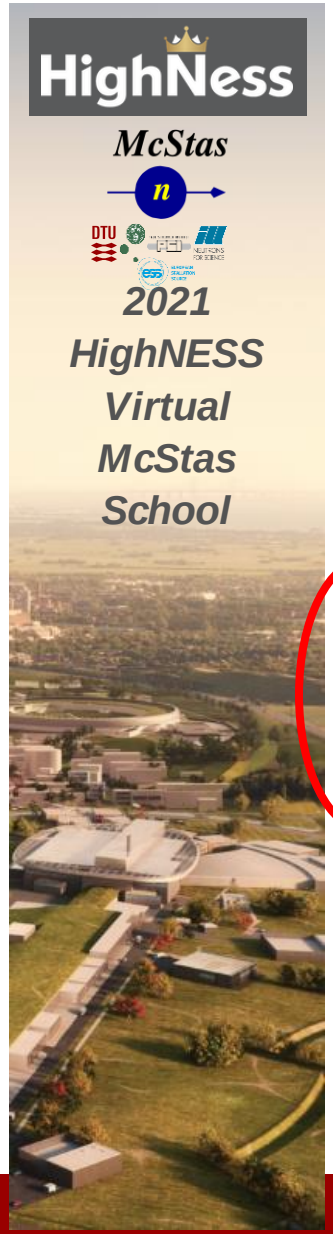


Single Crystal model

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 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

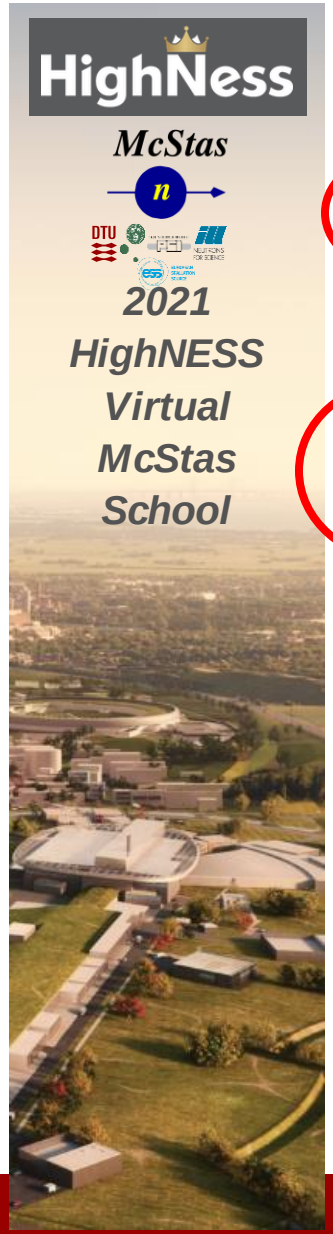
Input parameters

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 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 o		0
cy			0
cz			0
p_transm	1		-1
sigma_abs	barns		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

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

Single Crystal



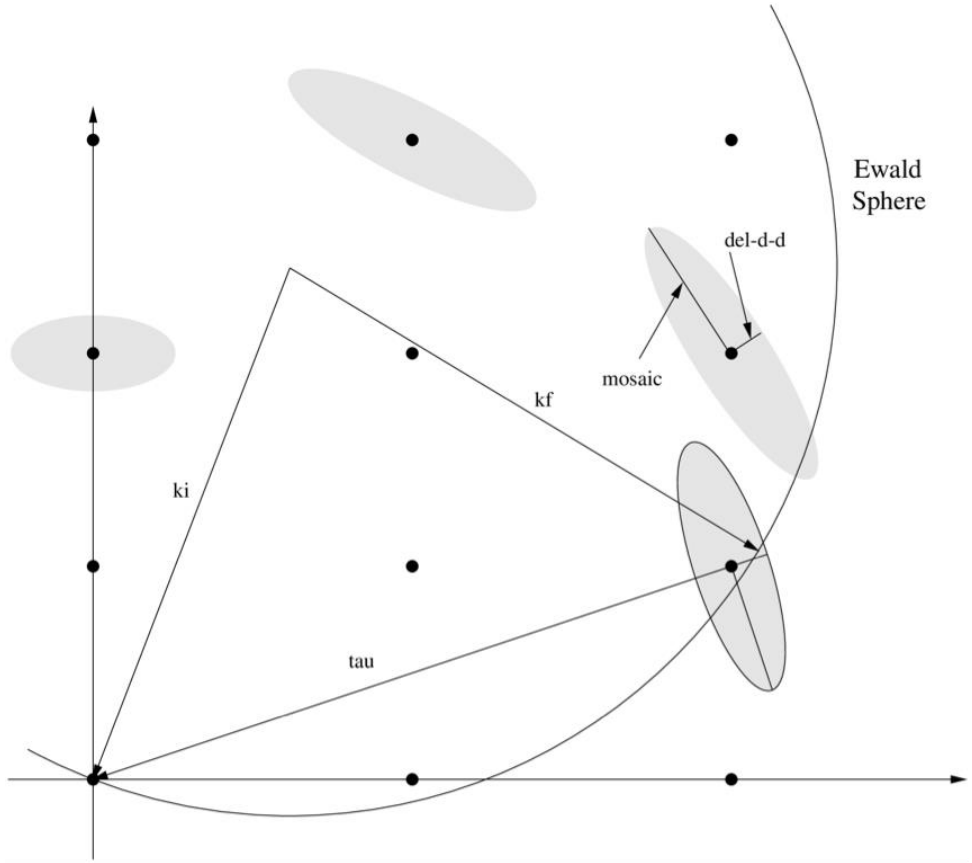
Input parameters

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 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		1e-4
mosaic	arc minutes		-1
mosaic_a	arc minutes	ors. Has precedence over in-plane mosaic model.	-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

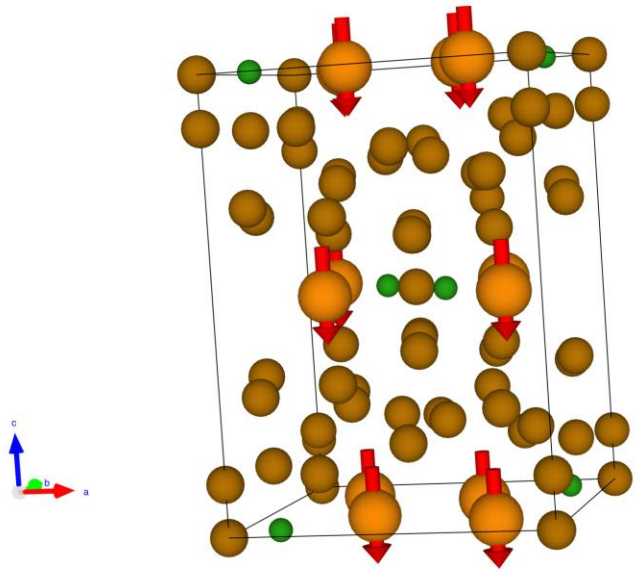
Single crystal mosaicity

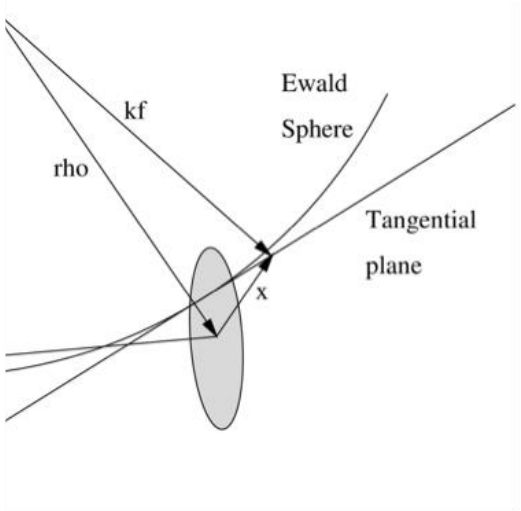


Single Crystal mosaicity

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.

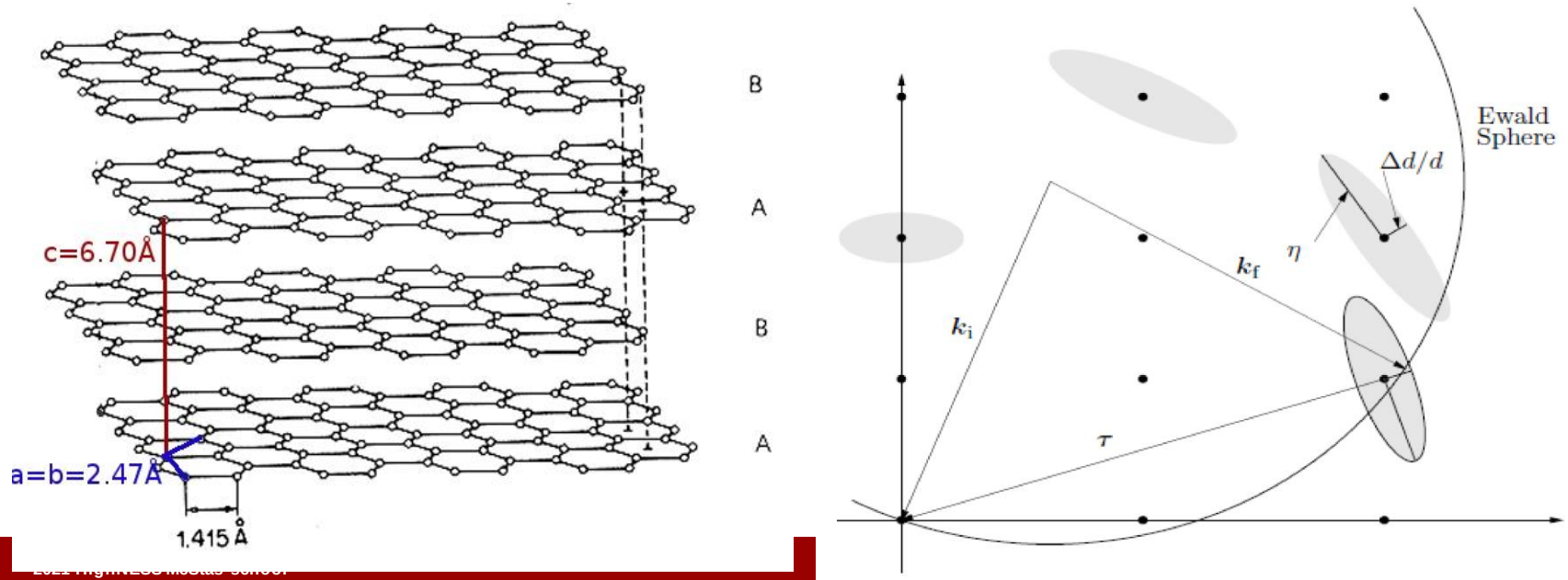


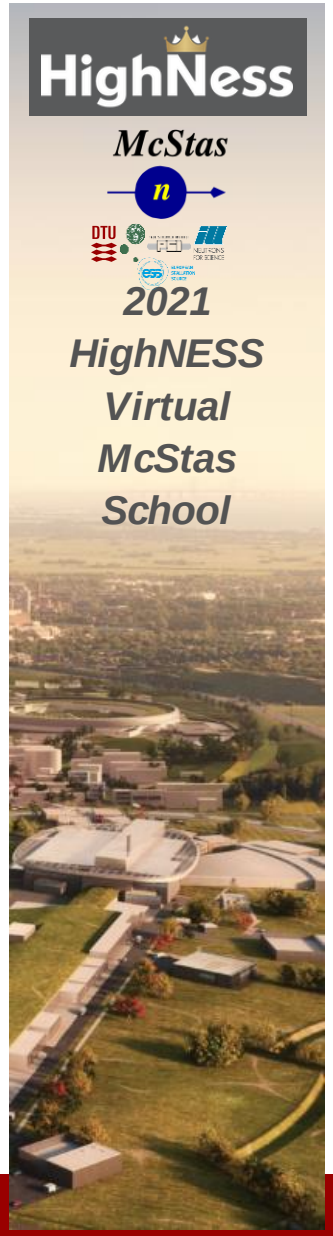


Single Crystal mosaicity

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 &sigma, and hkl for two peaks.



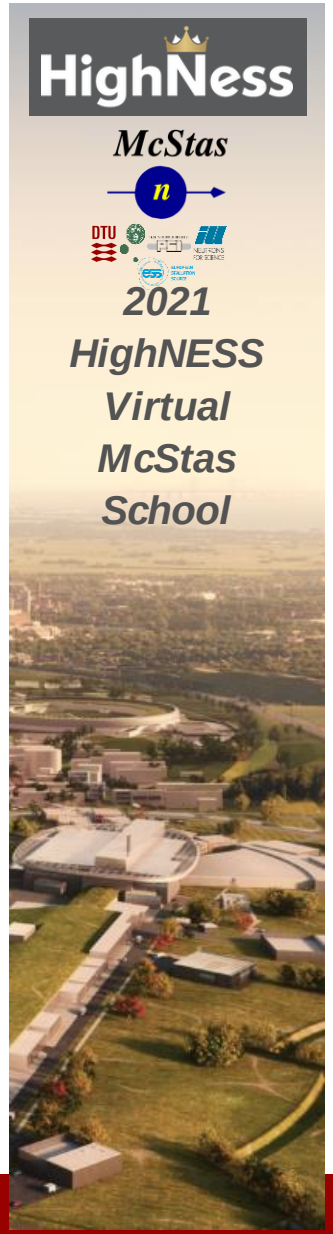


Exercise time!

Let's build a simplified Laue Camera and put a single crystal sample in it.

Head over to the github site and do Part 1.

9.2 PowderN



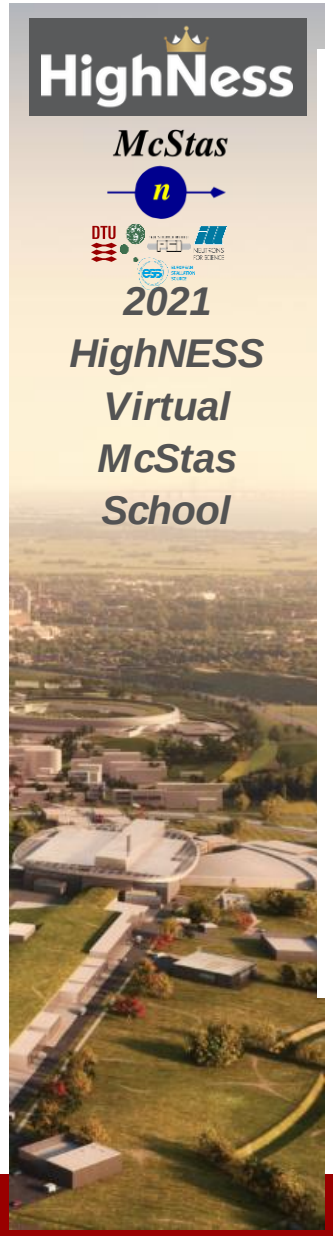
Among the most common materials measured with neutron scattering techniques are powders, which are composed of a large number of tiny single crystals. The scattering intensity, by means of constructive interference and averaging over all crystallites, appears as well defined rings around the out-going 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,

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

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

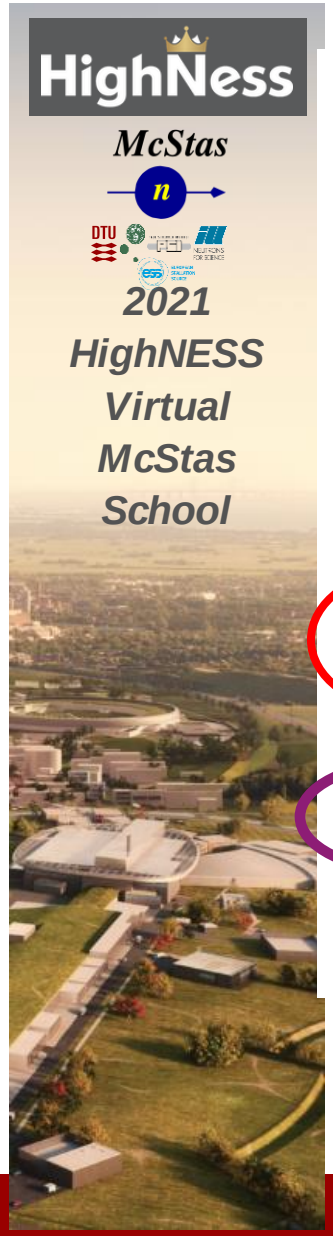


Input parameters

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



Input parameters

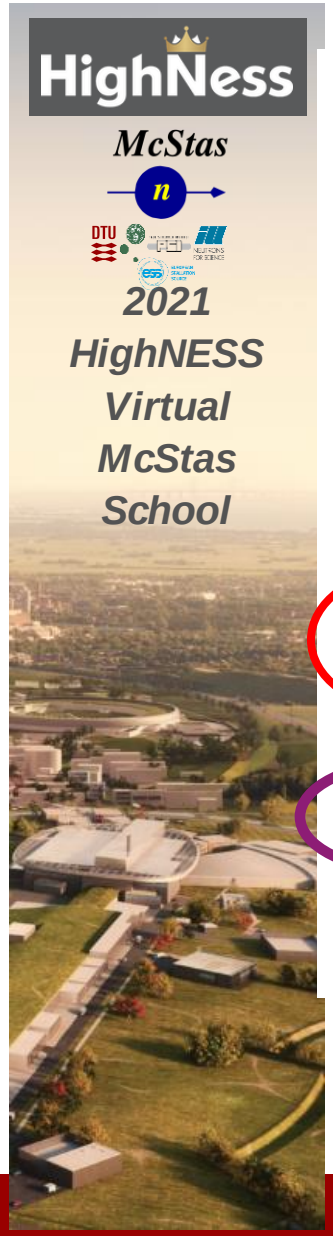
Parameters in **boldface** are required; the others are optional.

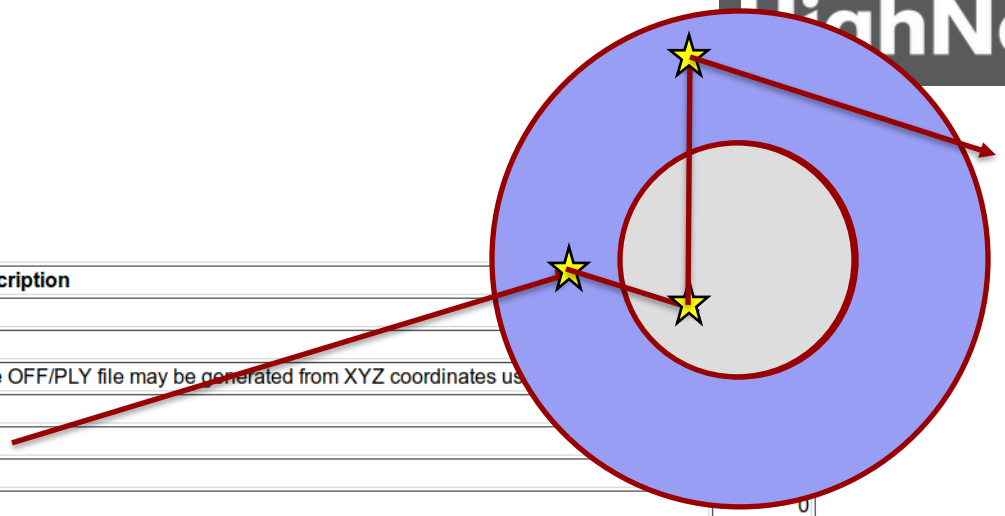
Name	Unit	Description	Default
format	no quotes	Name of the format, or list of column indexes (see Description).	Undefined
reflections			"NULL"
geometry	str	Name of an Object File Format (OFF) or PLY file for complex geometry. The OFF/PLY file may be generated from XYZ coordinates using qhull/powercrust	"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	…n the 'w' column is not available. Use 0 if ideal.	0
p_inc	1	…ays	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

Sampling parameters

Concentric = Hollow
Powder [cylinder]

PowderN inputs





Input parameters

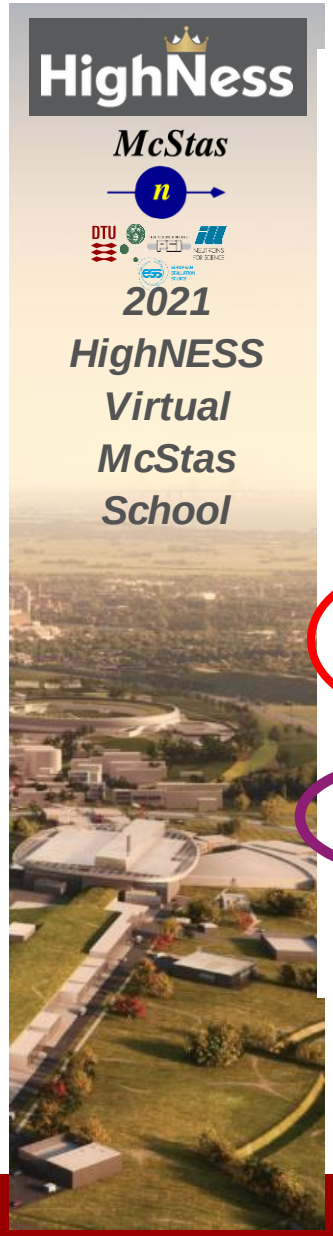
Parameters in **boldface** are required; the others are optional.

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	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	en the 'w' column is not available. Use 0 if ideal.	0
p_inc	1	ays	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

Sampling parameters

Concentric = Hollow
Powder [cylinder]

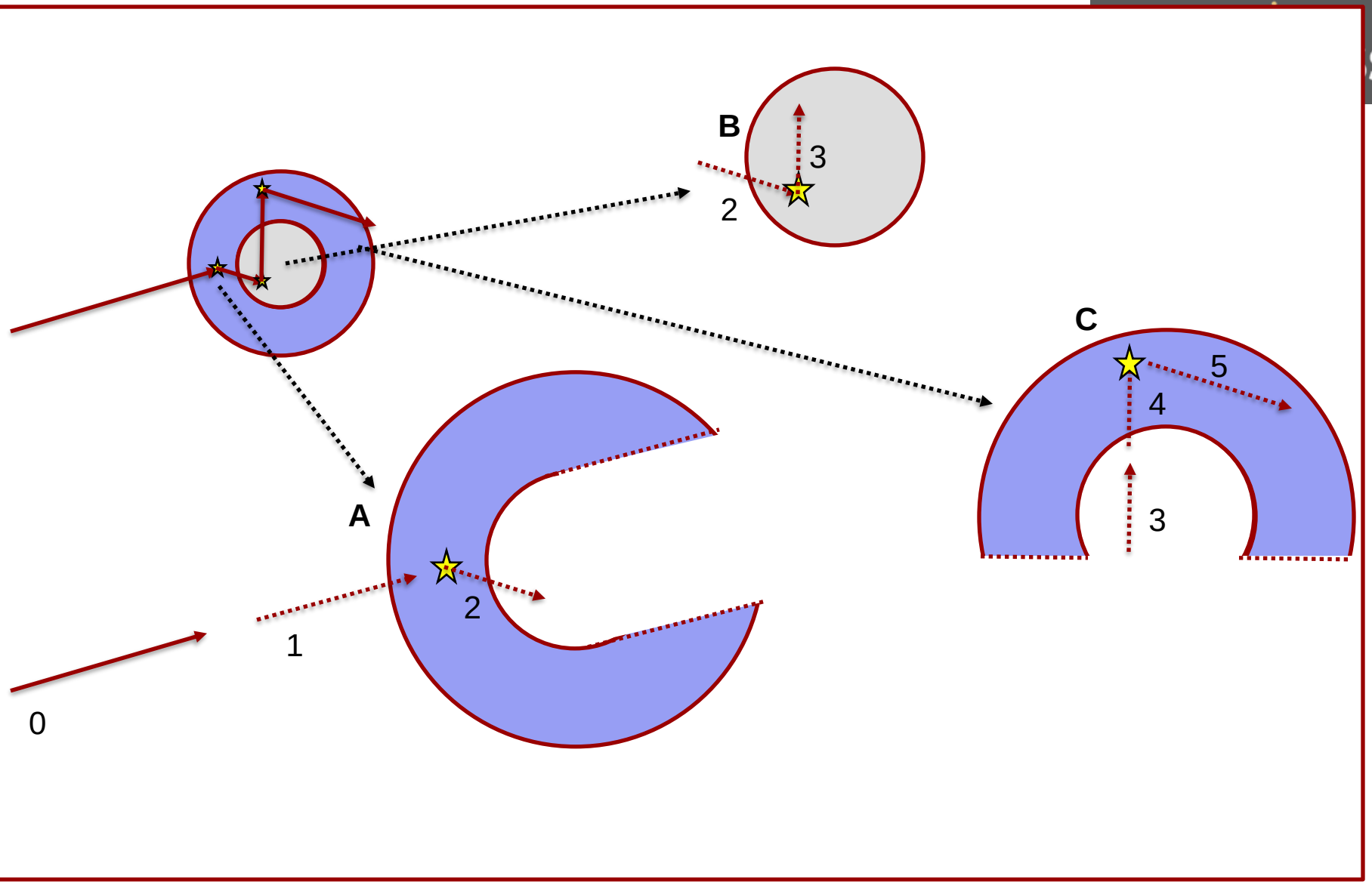
Powderl



Input parameters

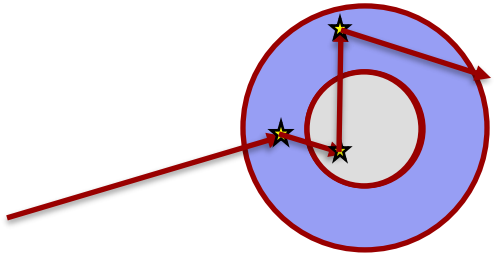
Parameters in **boldface** are re

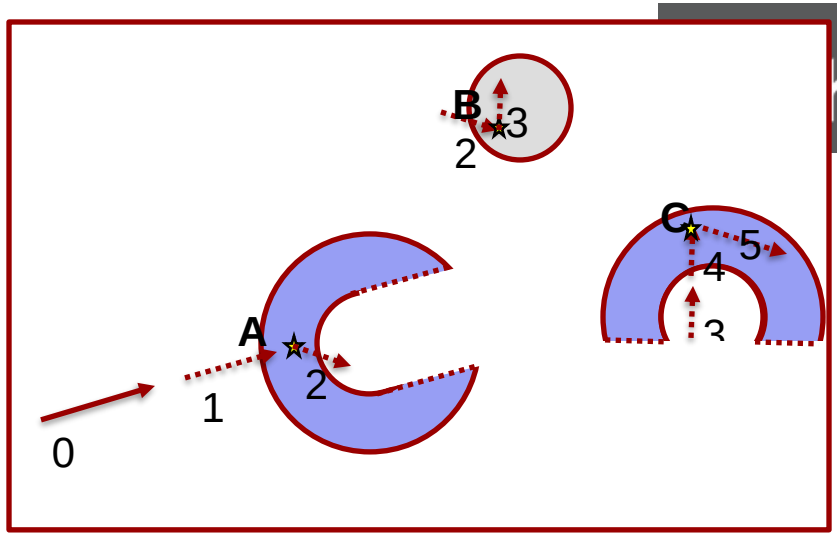
Name	Unit
format	no quotes
reflections	
geometry	str
radius	m
yheight	m
xwidth	m
zdepth	m
thickness	
pack	1
Vc	AA^3
sigma_abs	barns
sigma_inc	barns
delta_d_d	0/1
p_inc	1
p_transmit	1
DW	1
nb_atoms	1
d_phi	deg
p_interact	
concentric	only for box, cylin
density	g/cm^3
weight	g/mol
barns	1
Strain	ppm
focus_flip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



Concentric = Hollow
Powder [cylinder]

PowderN concentric in code



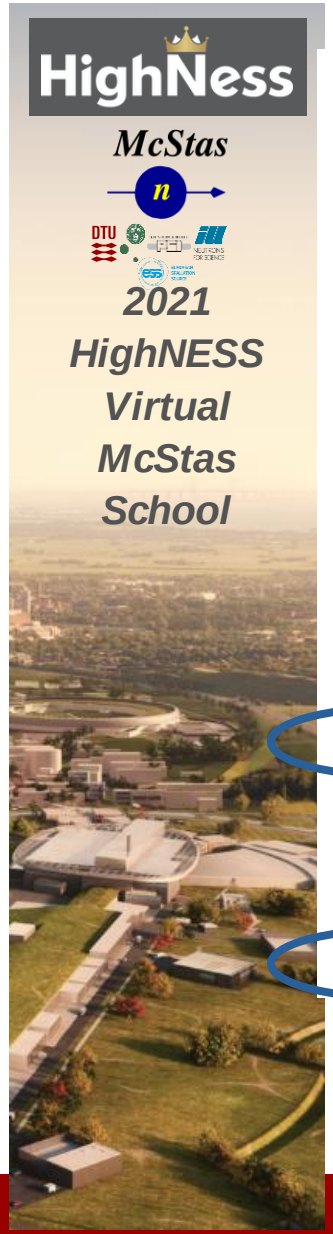



```
COMPONENT Al = PowderN(
    reflections="Al.laz", radius=0.02, yheight=0.05,
thickness=0.005,
    p_transmit=0.8, concentric=1)
AT (0, 0, 0) RELATIVE PREVIOUS

COMPONENT al2co3 = 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



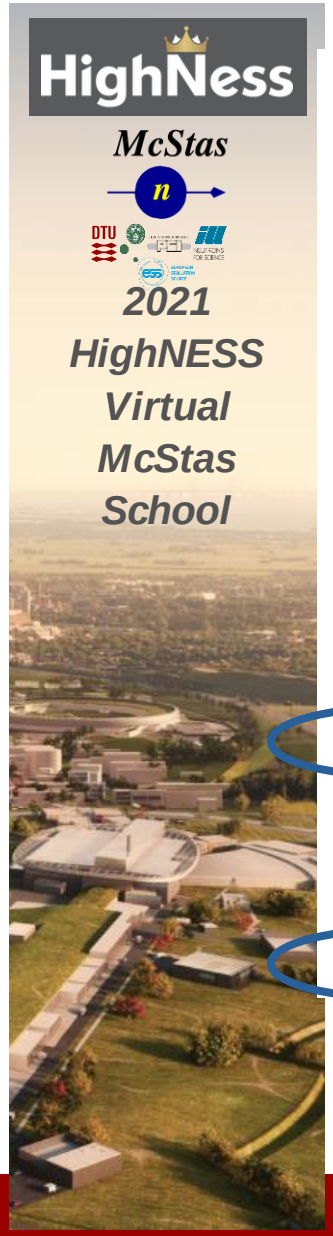
Input parameters

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

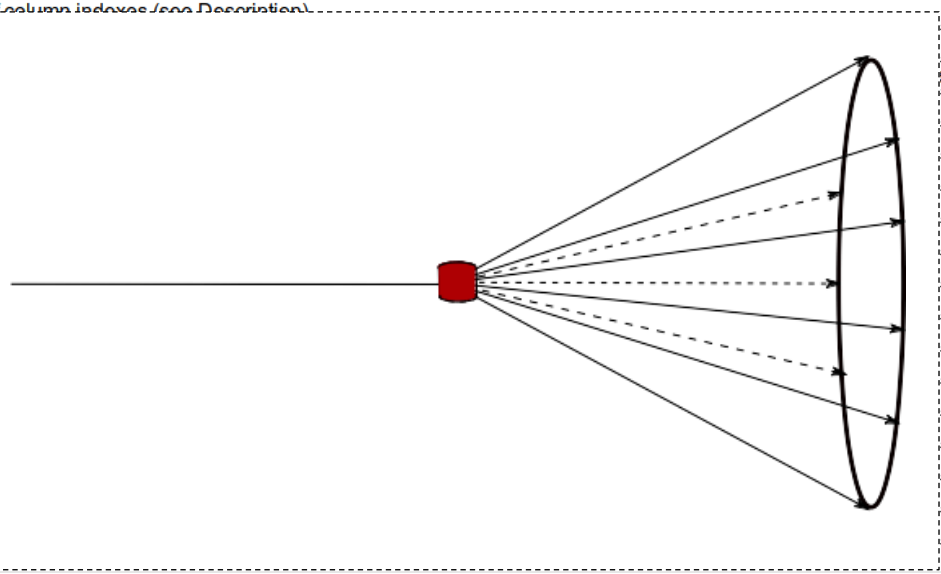
PowderN inputs



Input parameters

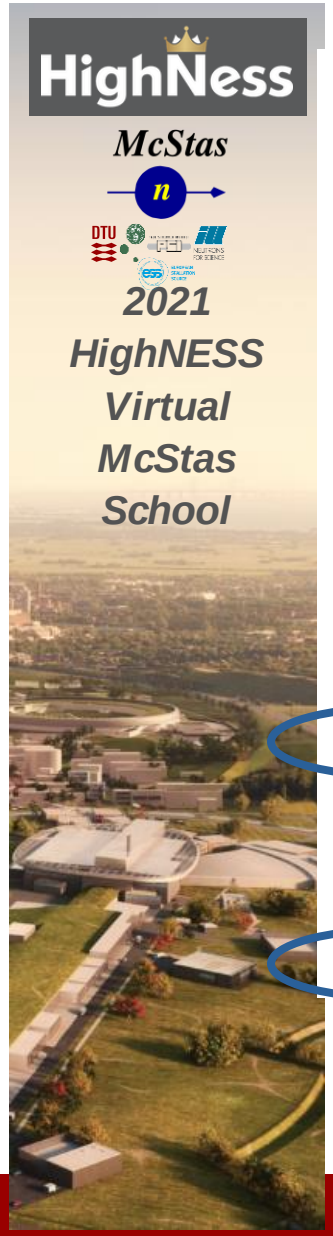
Parameters in **boldface** are required; the others are optional.

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 F	"NULL"
radius	m	Outer radius of sample in	0
yheight	m	Height of sample y directi	0
xwidth	m	Horiz. dimension of samp	0
zdepth	m	Depth of box sample	0
thickness			0
pack	1	Packing factor	1
Vc	AA^3	Volume of unit cell=nb at	0
sigma_abs	barns	Absorption cross section	0
sigma_inc	barns	Incoherent cross section	0
delta_d_d	0/1	Global relative delta_d_d	0
p_inc	1	Fraction of incoherently s	0.1
p_transmit	1	Fraction of transmitted (o	0.1
DW	1	Global Debye-Waller fact	0
nb_atoms	1	Number of sub-unit per u	1
d_phi	deg	Angle corresponding to th	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 4\pi

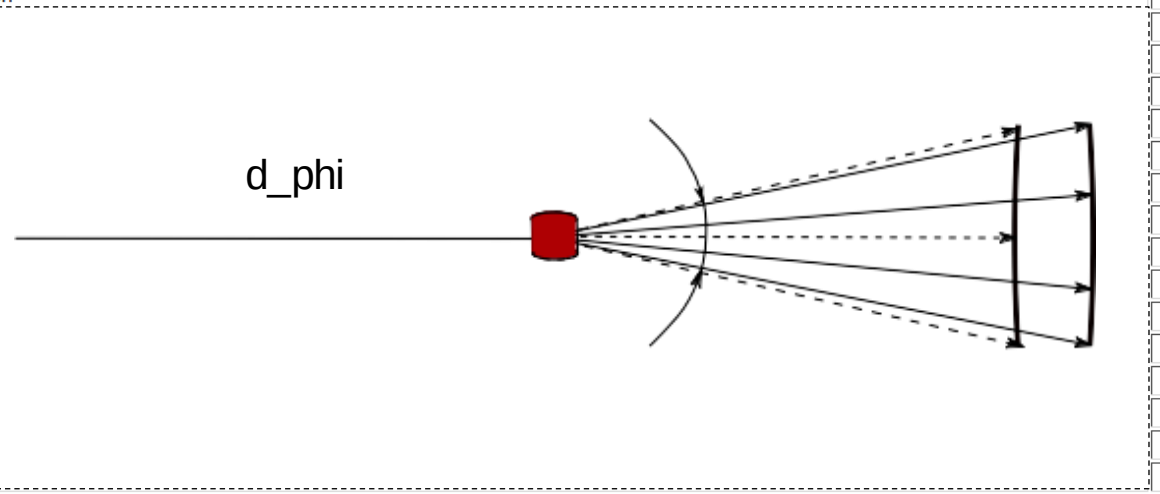
PowderN inputs



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 s	0
zdepth	m	Depth of box sample	0
thickness			0
pack	1	Packing factor	1
Vc	AA^3	Volume of unit cell=r	0
sigma_abs	barns	Absorption cross sec	0
sigma_inc	barns	Incoherent cross sec	0
delta_d_d	0/1	Global relative delta	0
p_inc	1	Fraction of incoheren	0.1
p_transmit	1	Fraction of transmitte	0.1
DW	1	Global Debye-Waller	0
nb_atoms	1	Number of sub-unit p	1
d_phi	deg	Angle corresponding	0
p_interact	1	Fraction of events int	0
concentric	only for box, cylinder, sphere	[1] Indicate that this c	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 4\pi

Reflection files for Single_crystal and PowderN

```
# TITLE *Aluminum-Al-[FM3-M] Miller, H.P.jr.;DuMond, J.W.M.[1942] at 298 K
# 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]
# w eight 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]
# column_F2 7 norm of scattering factor |F|^2 in [fm^2]
# column_h 1
# column_k 2
# column_l 3
#
# h k l Mult. d-space 2Theta F-squared
-1 -1 -1 8 2.338 24.6973 21.3
-1 -1 1 8 2.338 24.6973 21.3
…
```

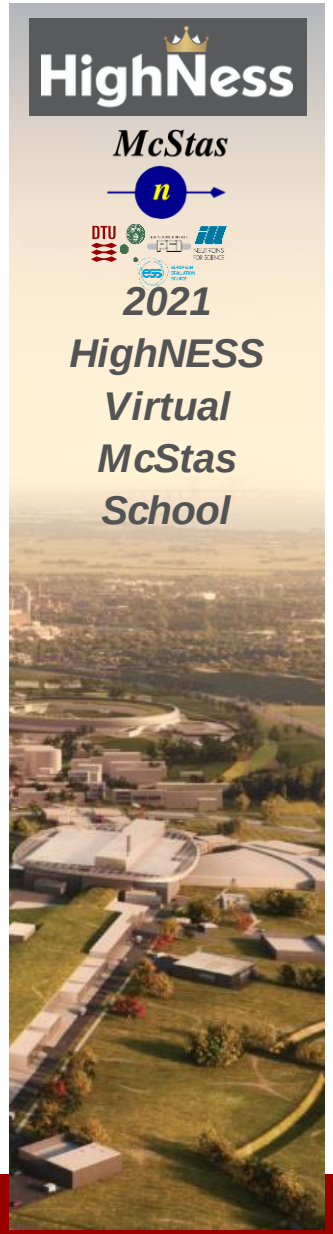
Lau datafiles

header

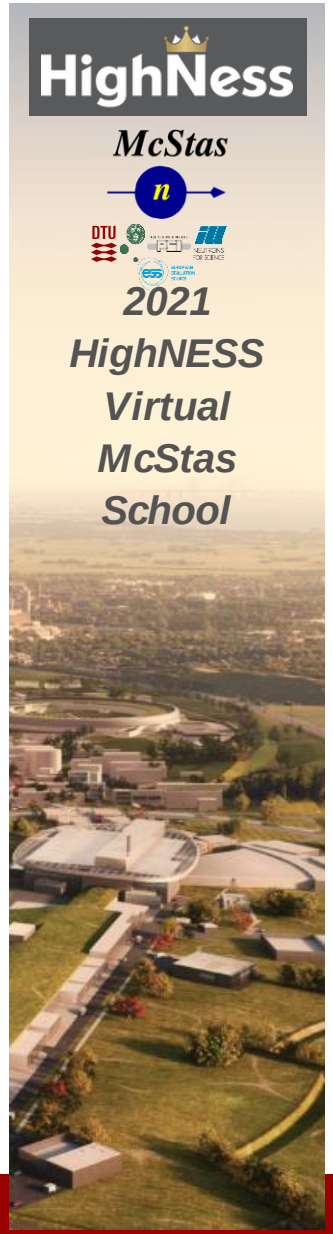
+

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
# column_k 2
# column_l 3
#
# H  K  L  THETA  2THETA  D VALUE  1/D**2 SIN2*1000  H  K  L INTENSITY          /F(HKL)/     A(HKL)     B(HKL) PHA.ANG. MULT   LPG
  1  0  1  6.35   12.71   4.5175   0.0490    12.25   1  0  1      367.0           4.1          -4.08                0.00 180.00  6  82.14
  0  0  3  7.10   14.20   4.0467   0.0611    15.27   0  0  3      110.0           4.3           4.32                0.00   0.00  2  66.01
  0  1  2  7.57   15.13   3.7972   0.0694    17.34   0  1  2       10.9           0.8           0.84                0.00   0.00  6  58.18
...
```

Laz + Lau datafiles

header

+

reflection list

Can be used with PowderN, Isotropic_Sqw

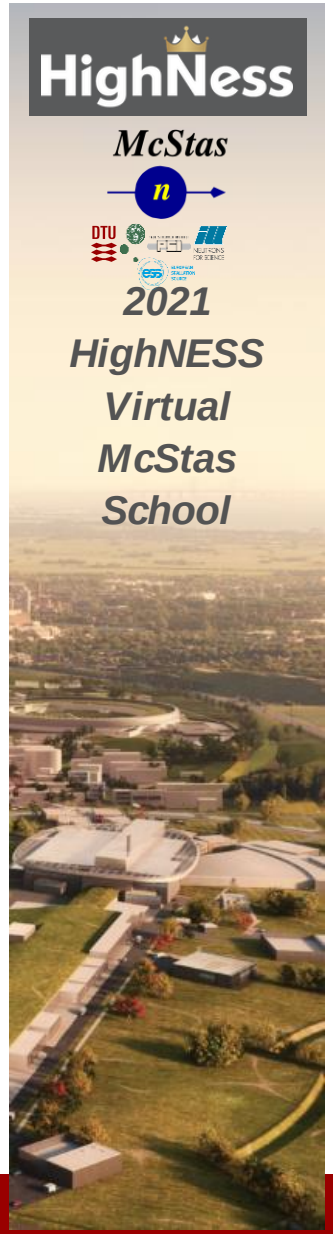
What's already there?

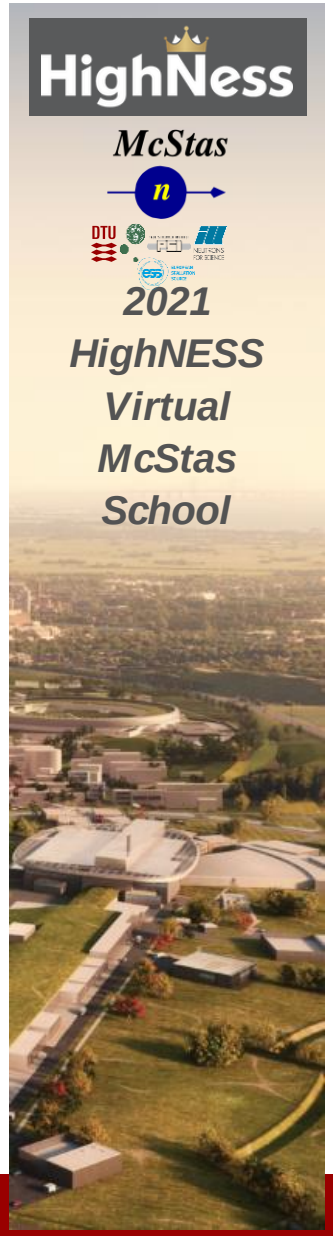
Single Crystals

Al.lau
Al2O3_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
SiO2_cristobalite.lau
SiO2_quartza.lau
SiO2_quartzb.lau
TiO2_rutile.lau
YBaCuO.lau
adrenaline.lau
aspirin.lau
leucine.lau

Powders

Ag.laz
Al.laz
Al2O3_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
SiO2_quartza.laz
SiO2_quartzb.laz
Sn_alpha.laz
Sn_beta.laz
Ti.laz
Tl.laz
UO2.laz
V.laz
Y2O3.laz
Y3Fe5O12_YIG.laz
Zn.laz

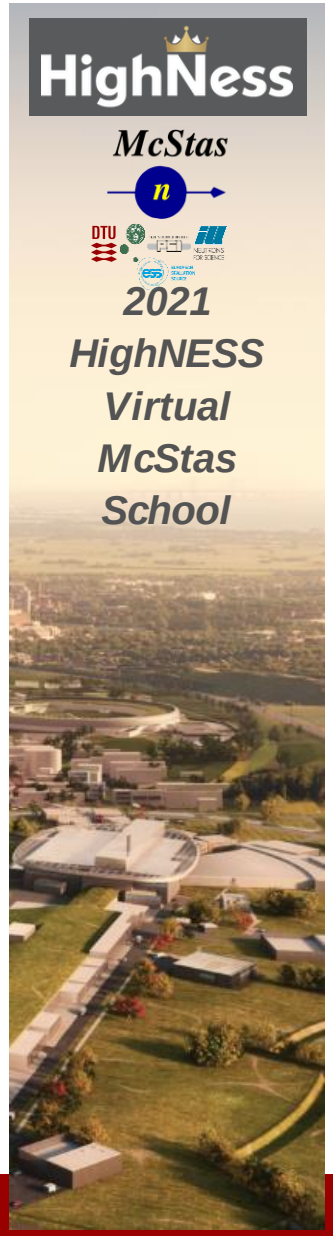




Where to get these files…

- $MCSTAS/data
  - Windows: c:\mcstas-3.0\lib\data
  - Linux: /usr/(local)/share/mcstas/3.0/data
  - OS X: /Applications/McStas-3.0/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>
  - Process it using
    - cif2hkl which is available in your McStas installation



https://github.com/McStasMcXtrace/McCode/wiki/Generating-input-files-for-Single_crystal-and-PowderN

https://github.com/McStasMcXtrace/McCode/wiki/Generating-input-files-for-Single_

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Unwatch 12 Star 44 Fork 38

Code Issues 197 Pull requests Actions Projects 10 Wiki Security Insights Settings

Generating input files for Single_crystal and PowderN

Edit New Page

Peter Willendrup edited this page 17 days ago · 2 revisions

The main diffraction-oriented samples of the McStas- and McXtrace-packages are called Single_crystal and PowderN.

Both components take input files in the form of reflection lists defining the crystallographic information, these can often be generated from a CIF file using the "cif2hkl" command line utility included with your McStas or McXtrace installation. The below example commands are run with --mode NUC for nuclear scattering / neutrons, please use --mode XRA for X-ray scattering.

To generate a file with a PowderN-compatible reflection list for McStas, use e.g.

```
cif2hkl --powder --mode NUC MnO_Fm-3m.cif -o MnO_Fm-3m.hkl
```

(The "--powder" or "-p" parameter will put one line per a set of equivalent reflections, i.e. only positive (h k l) indexes. This file type of file is therefore NOT compatible with Single_crystal.)
To generate a file with a Single_crystal and PowderN-compatible reflection list for McStas, use e.g.

```
cif2hkl --xtal --mode NUC MnO_Fm-3m.cif -o MnO_Fm-3m.hkl
```

(The "--xtal" or "-x" parameter will lists all reflections, including equivalent ones with signed (h k l) indexes, as needed by Single_crystal. Please note that the hkl sorted with respect to increasing length of the scattering vector.)
The crystallographic input-files distributed with McStas are typically found in either .laz powder-format (e.g. Si.laz as example) or .lau single-crystal-format (e.g. YBaCuO.lau) that content-wise are close to what one would get from the above cif2hkl example runs, but with different order of the columns in the reflection lists.

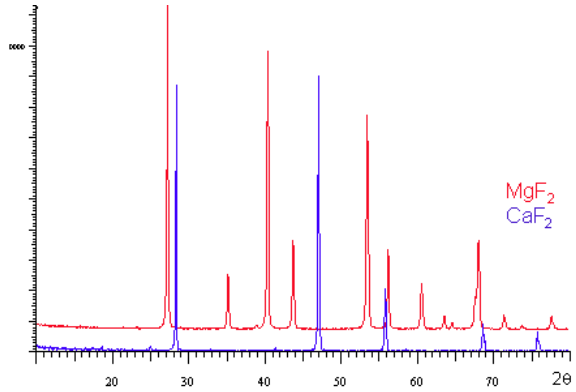
Pages 48

Find a Page...

- Home
- 2020 Virtual McStas McXtrace GPU hackathon (November)
- Access to the code tree
- Building McStas McXtrace
- Builds and platforms overview
- Changes and differences between McStas 2.x and 3.0
- Debugging the c code
- Developer literature
- Generate Vitess modules via mcstas2vitess
- Generating input files for Single_crystal and PowderN
- GPUhack building and installing McStas

McStas: structure: powder

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



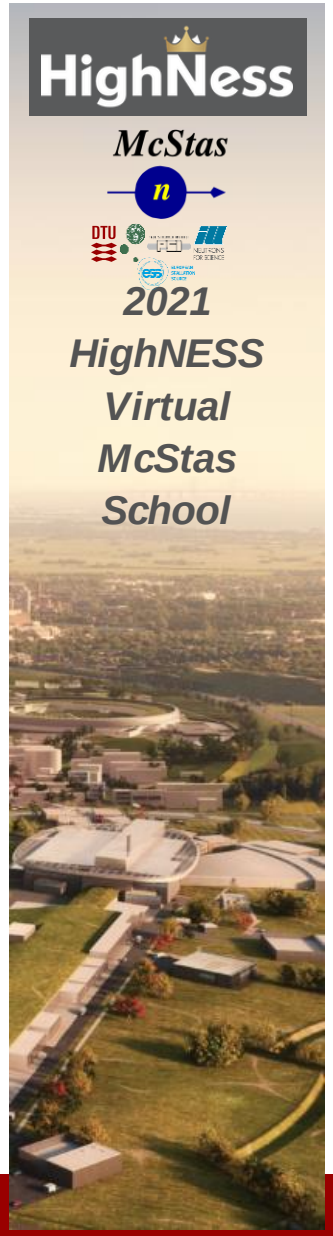
CIF file

FullProf/ShelX

Terminal:

```
cif2hkl --powder
file.cif
```

McStas Laz file



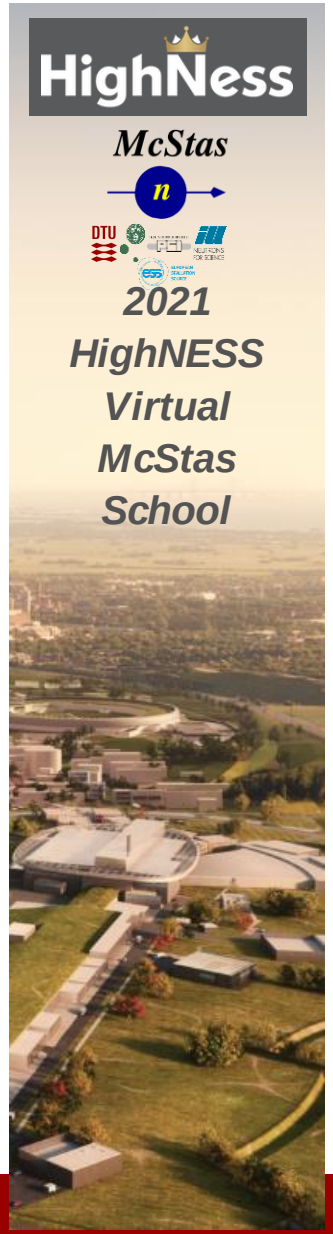
McStas: structure: SX

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

CIF file → Terminal: → McStas Lau file

FullProf/ShelX

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



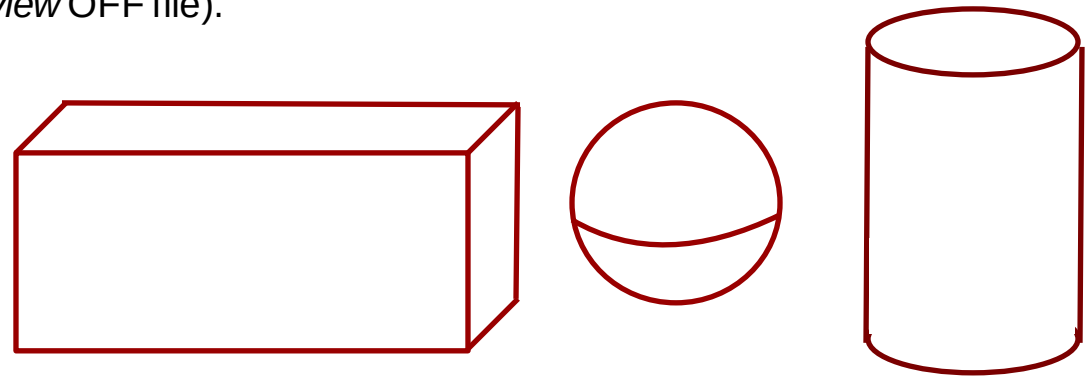
McStas Data formats

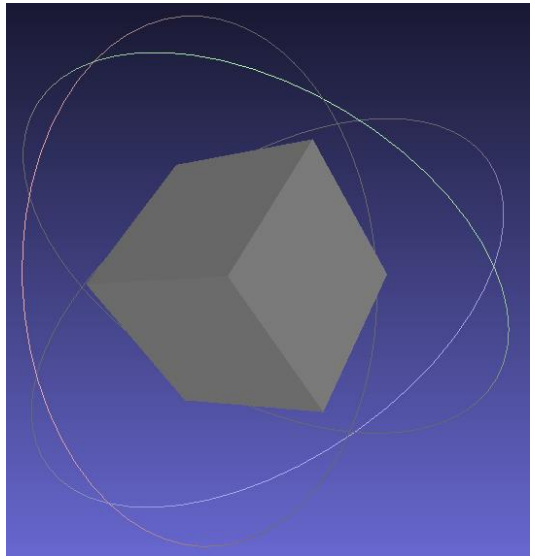
McStas uses a number of input data formats, all text based.

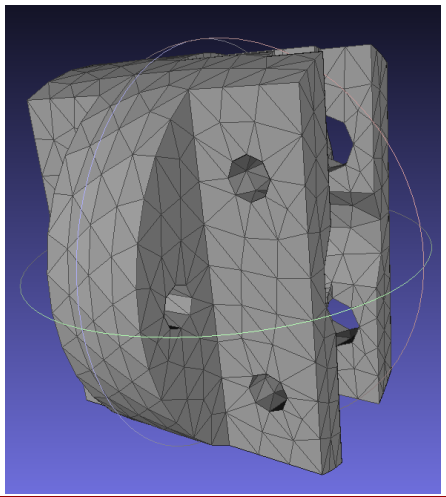
- **Lau** (Single_crystal, PowderN, Isotropic_Sqw)
- **Laz** (PowderN, Isotropic_Sqw)
- **Sqw** (Isotropic_Sqw)
- **qSq** (Isotropic_Sqw) – mostly for liquids
- **nxs** (Sample_nxs) – this is ***not*** a NeXus/HDF
- **PDB** (SANSPDB)
- **ncmat** (NCrystal)

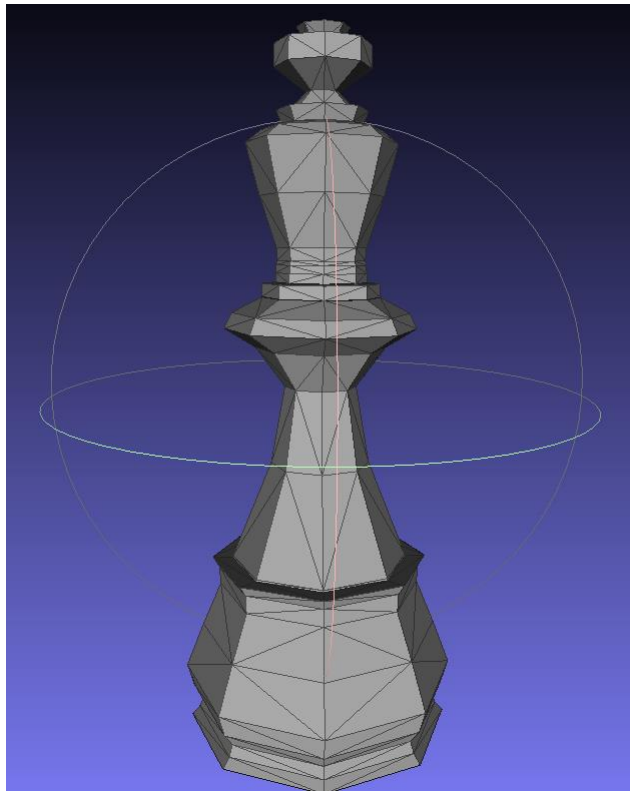
OFF/PLY any geometry

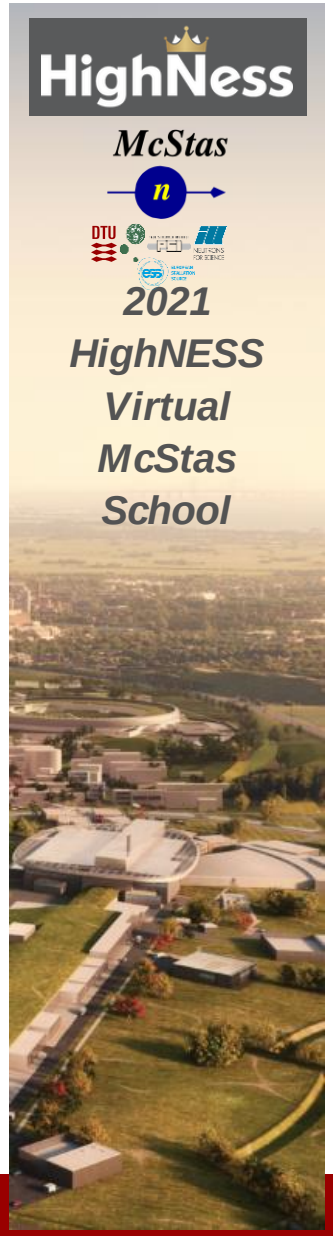
An additional complex geometry enables to use any point set to describe the material volume (*geomview* OFF file).











Exercise time!

Let's build a simplified Laue Camera and put a single crystal sample in it.

Head over to the github site and do Part 2.