



McStas



Erik Knudsen

Mctas samples for diffraction



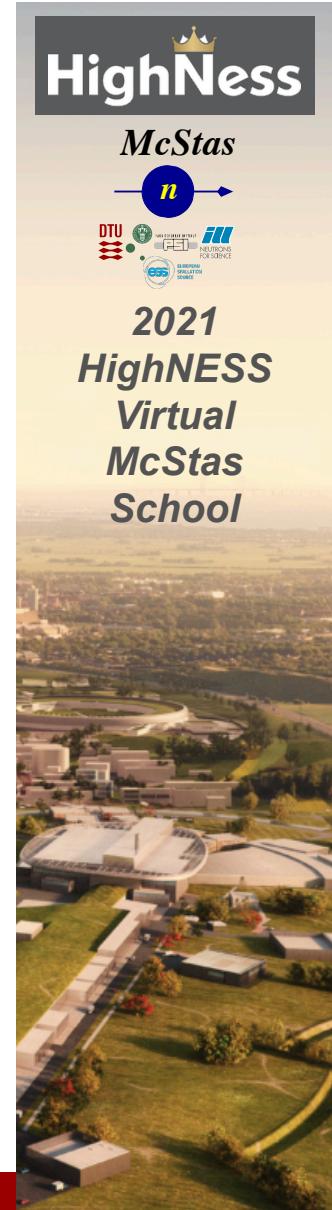
Agenda



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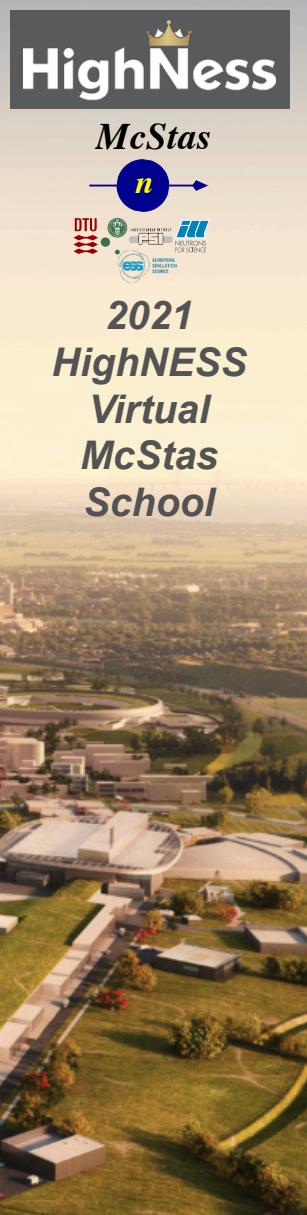


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- General concepts (reminder)
- Focus on diffraction-oriented samples:
 - Incoherent scatterer
 - Powder
 - Single Crystal
 - File formats

Add a slide on elastic scattering...



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Incoherent Sample

[Incoherent.comp](#)

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



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| 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 |

An incoherent scatterer with various sample shape options



Incoherent Sample

[Incoherent.comp](#)

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



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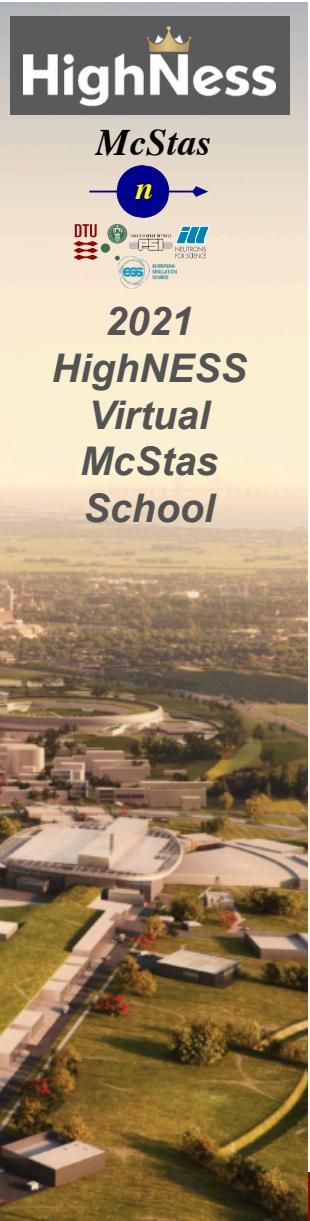
| Name | Unit | Description | Default |
|-------------------|-------|--|---------|
| geometry | str | Name of an Object File Format (OFF) or PLY file for complex geometry. The OFF/PLY file may be generated from XYZ coordinates using qhull/powercrust | 0 |
| radius | m | Outer radius of sample in (x,z) 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 peak | |
| 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





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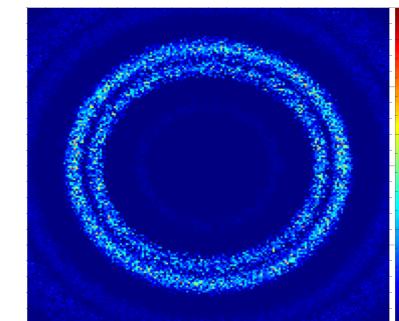
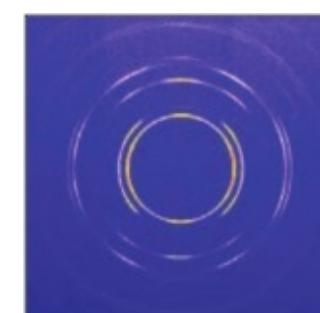
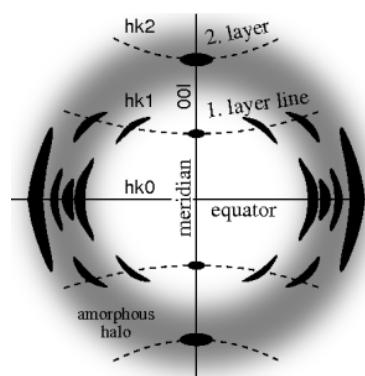
Single crystal



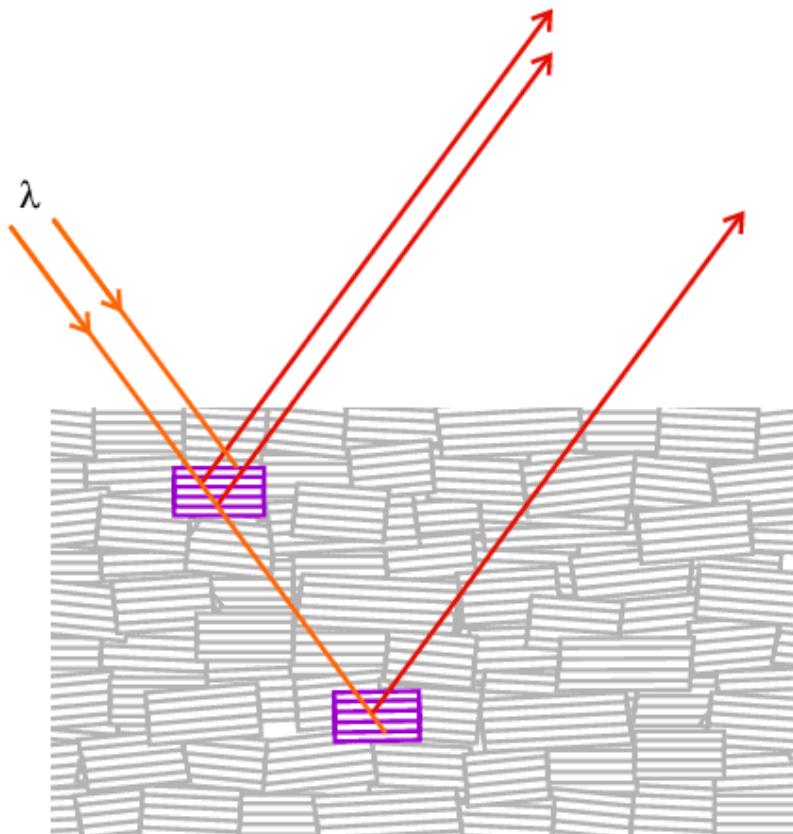
Polycrystal with a little disorder,
i.e. a *preferred orientation, texture*



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



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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 |



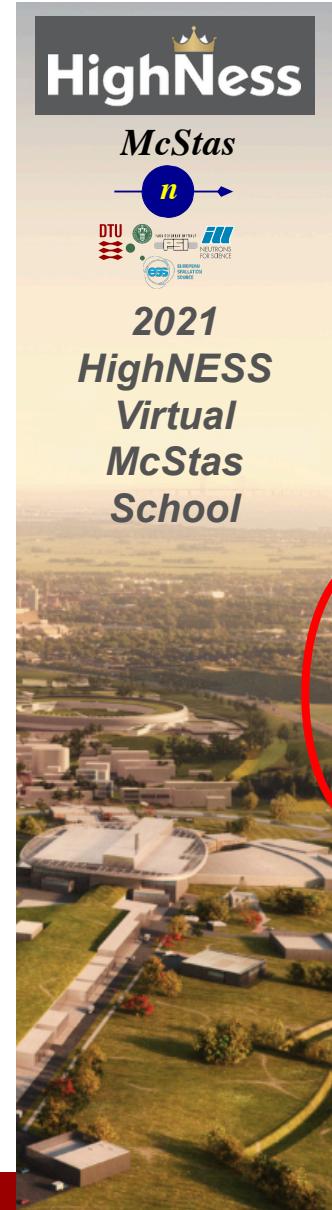
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Input parameters

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 |
| sigmida_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



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Input parameters

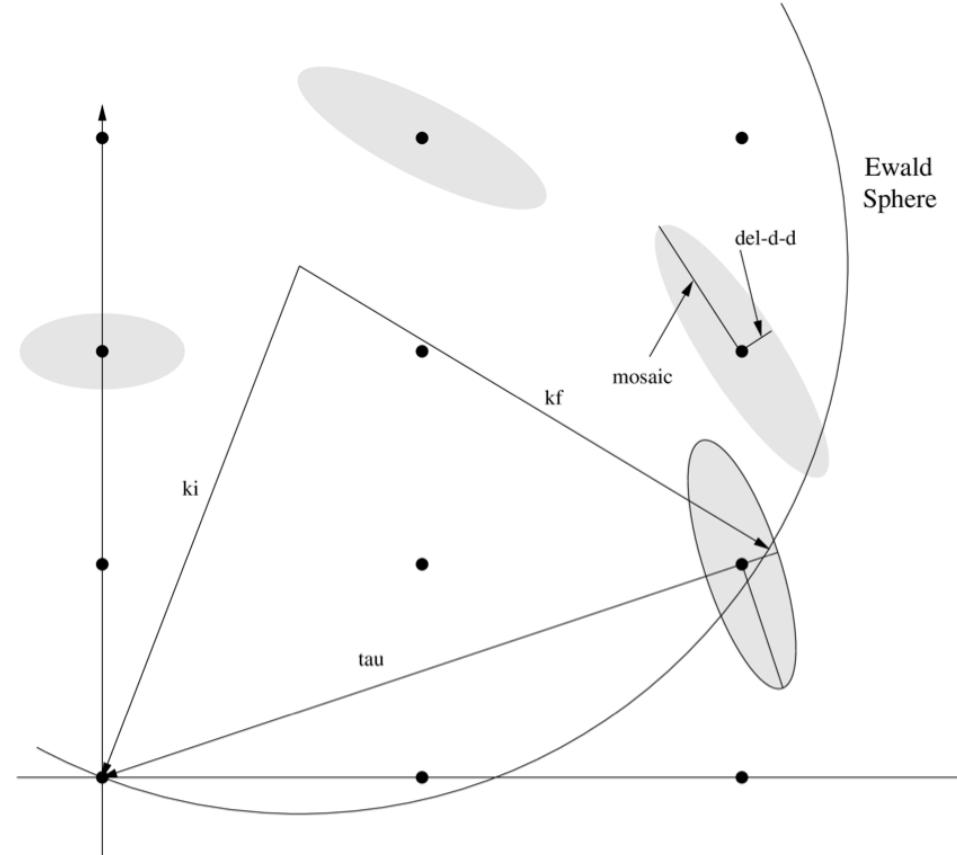
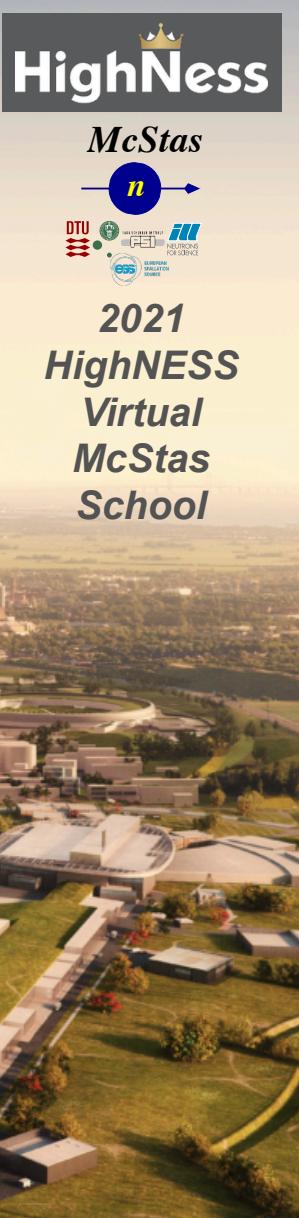
Parameters in **boldface** are required; the others are optional.

| Name | Unit | Description | Default |
|-------------|--------------------------------------|---|---------------------|
| mosaic_AB | arc_minutes, arc_minutes, 1, 1, 1, 1 | 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



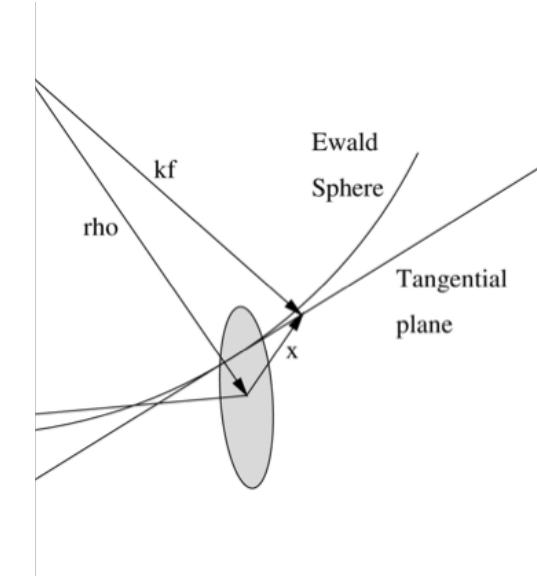
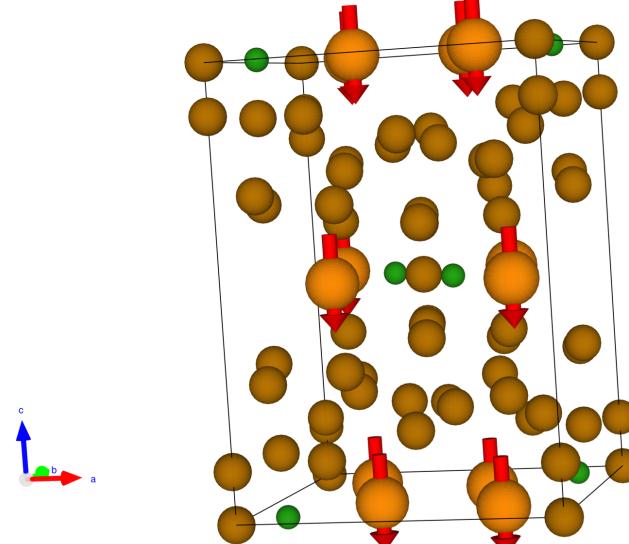
Single Crystal mosaicity



Single Crystal mosaicity

Three models:

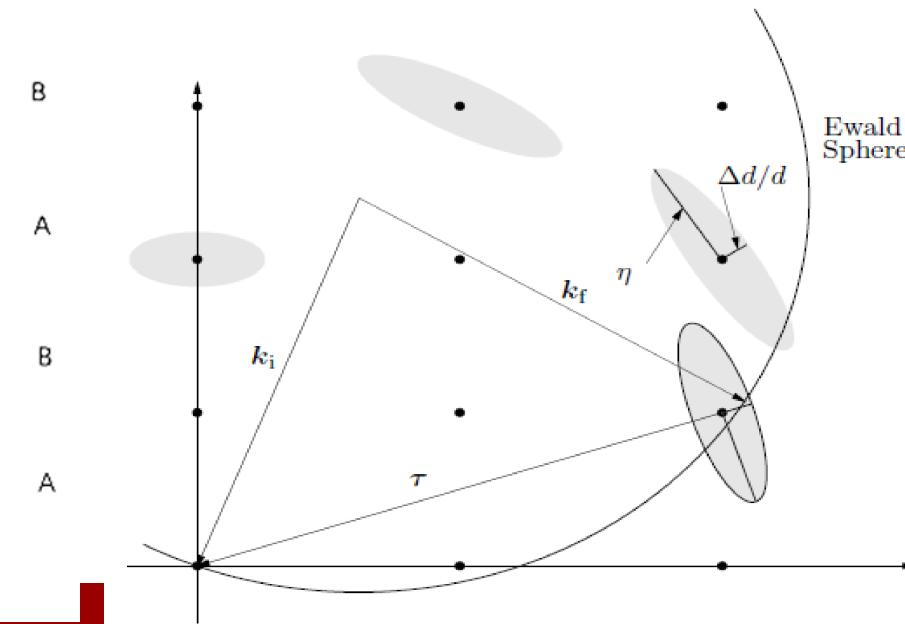
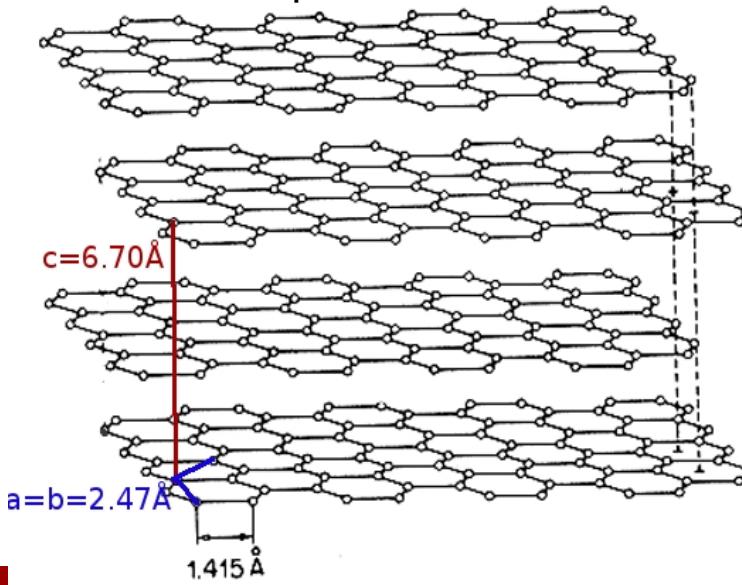
- Isotropic Mosaicity = Gaussian distribution of rotation angle, with given standard deviation, around a random vector.
- Anistropic mosaicity = Gaussian distribution of angles around each of the unit cell axis.



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

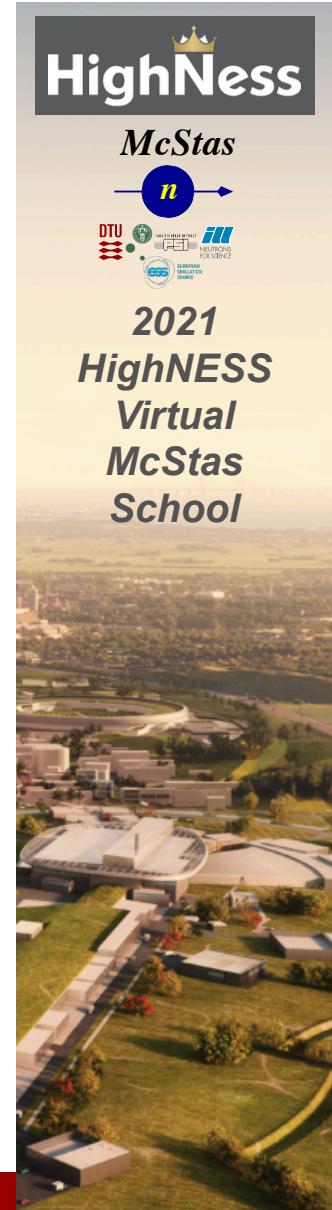


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Among the most common materials measured with neutron scattering techniques are powders, which are composed of a large number of tiny single crystals. The scattering intensity, by means of constructive interference and averaging over all crystallites, 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



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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 | 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



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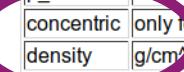
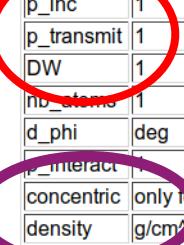
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Input parameters

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 | | 0 |
| p_inc | 1 | | 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 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



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Input parameters

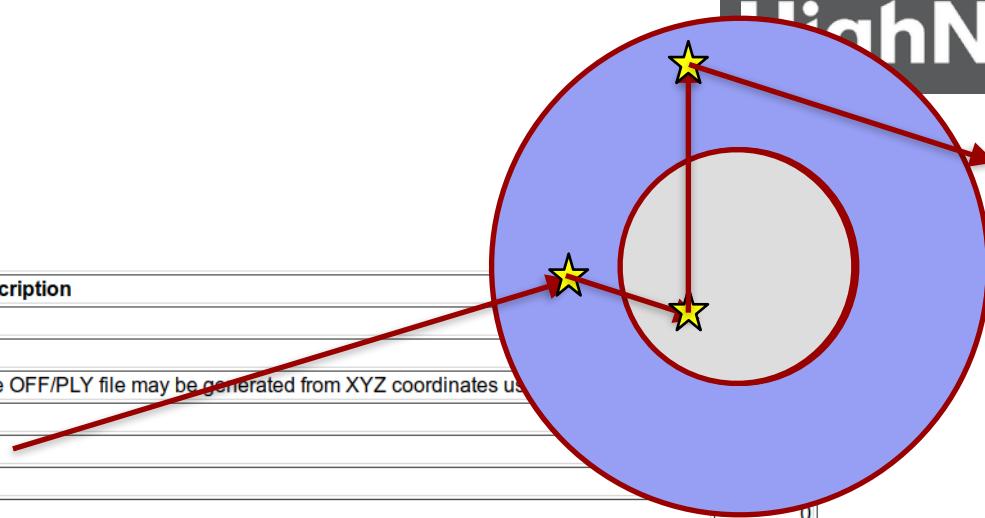
Parameters in **boldface** are required; the others are optional.

| 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 using the 'mcstas generate geometry' command. |
| 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_atoms | 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

| | | |
|------------|--------------------------------|---|
| 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_atoms | 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. |

Concentric = Hollow
Powder [cylinder]





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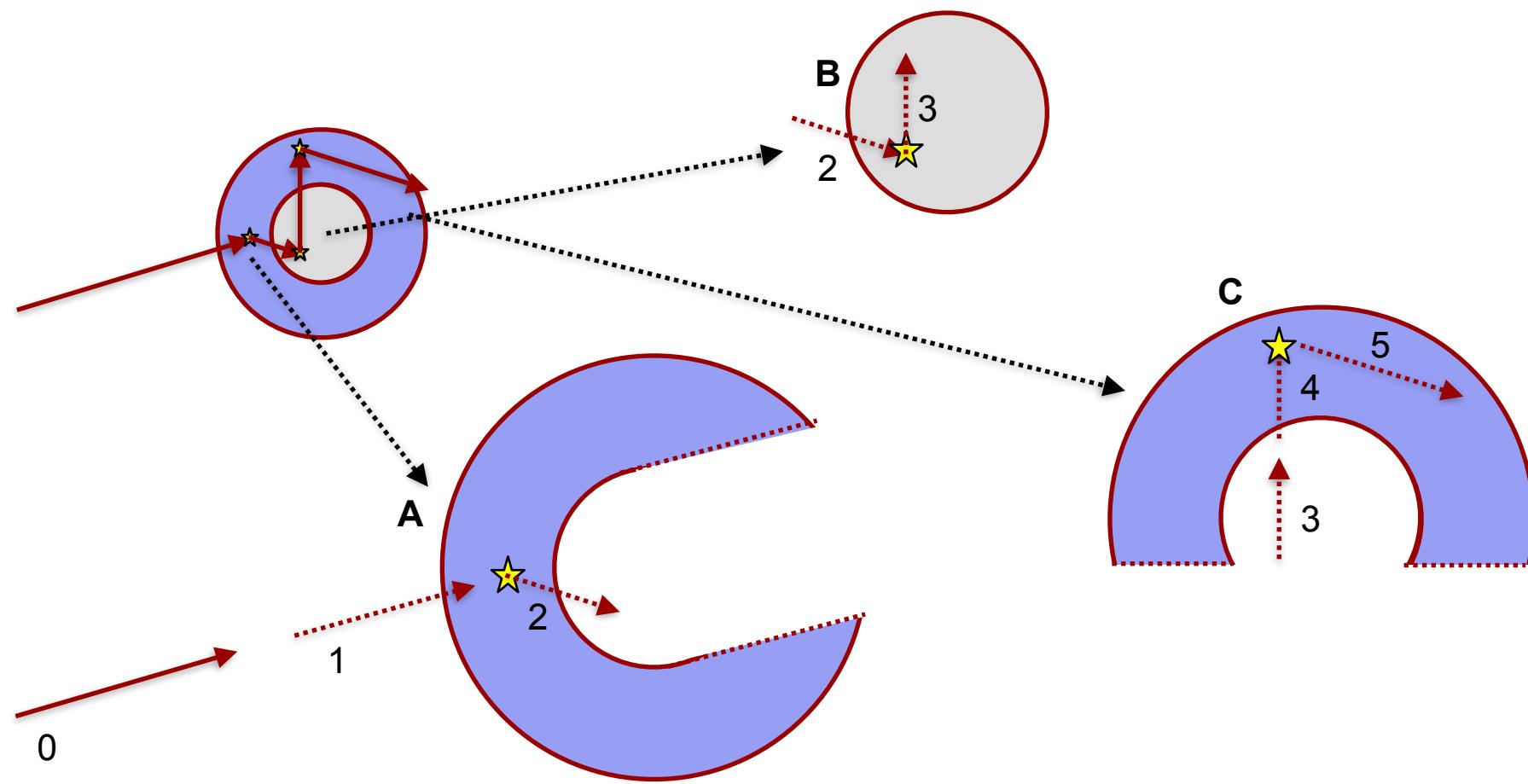


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Input parameters

Parameters in boldface are re

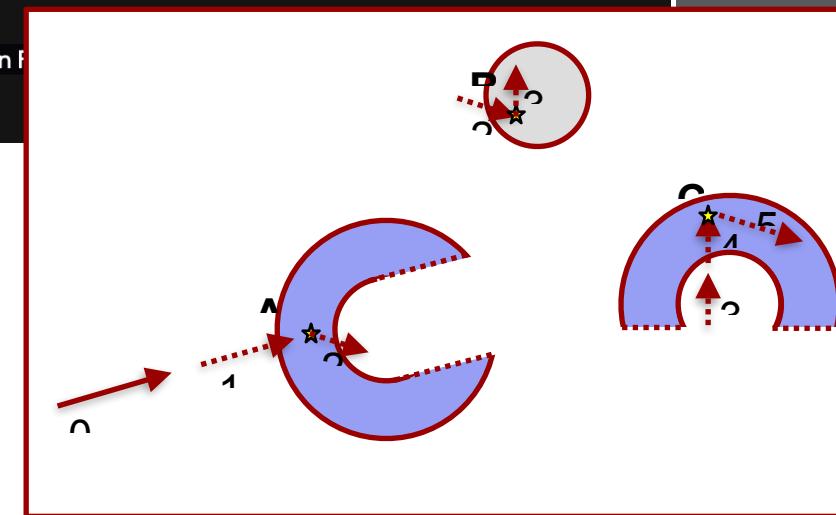
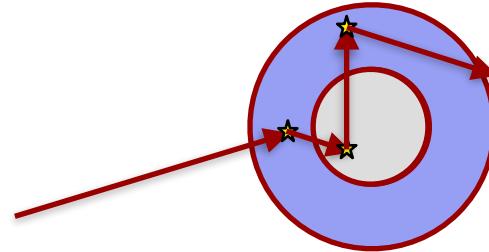
| Name | Unit |
|-------------------|------------------------|
| format | no quotes |
| reflections | |
| geometry | str |
| radius | m |
| yheight | m |
| xwidth | m |
| zdepth | m |
| thickness | |
| pack | 1 |
| Vc | AA^3 |
| sigma_abs | barns |
| sigma_inc | barns |
| delta_u_d | 0/1 |
| p_inc | 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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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



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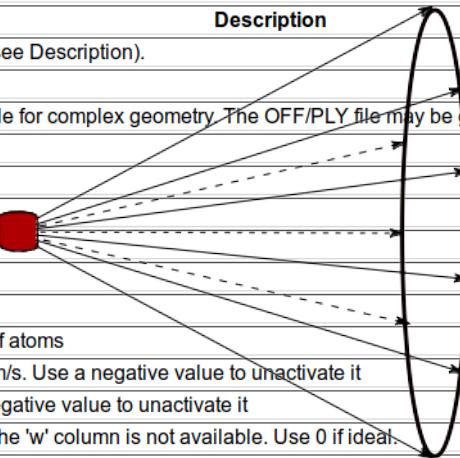
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Input parameters

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 |

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 4π



PowderN inputs



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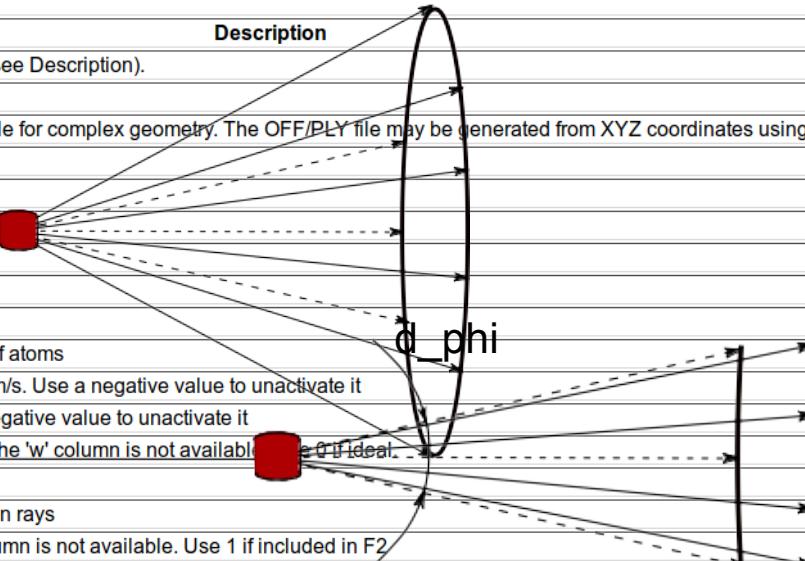
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Input parameters

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 |

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 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]
# c2021 HighNESS McStas school
```

scattering factor |F|^2 in [fm^2]



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Lau datafiles

header

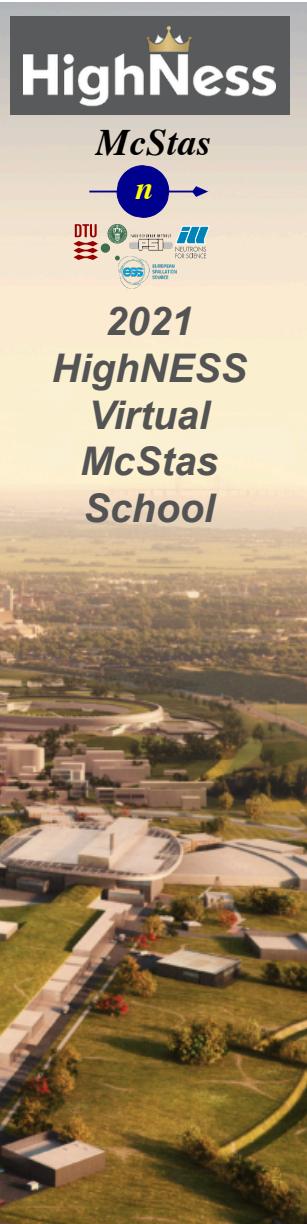
+

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]
2021 HighNESS McStas school
# column_h 1

```

Laz + Lau datafiles

header

+

reflection list

Can be used with PowderN,
Isotropic_Sqw





What's already there?

Single Crystals

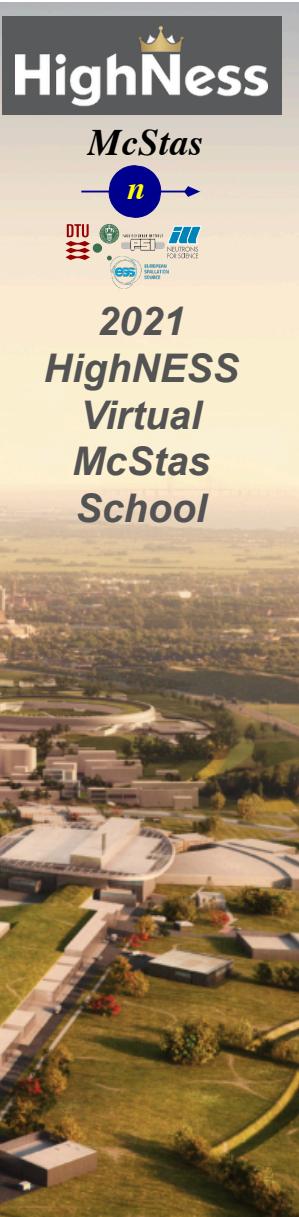
Al.lau
Al203_sapphire.lau
B4C.lau
BCC_fake.lau
BeO.lau
C60.lau
C_diamond.lau
C_graphite.lau
CaF2.lau
Ge.lau
In.lau
PPase_D_P1.lau
Rubredoxin.lau
Si02_cristobalite.lau
Si02_quartz.a.lau
Si02_quartzb.lau
Ti02_rutile.lau
YBaCu0.lau
adrenaline.lau
aspirin.lau
leucine.lau

Powders

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...

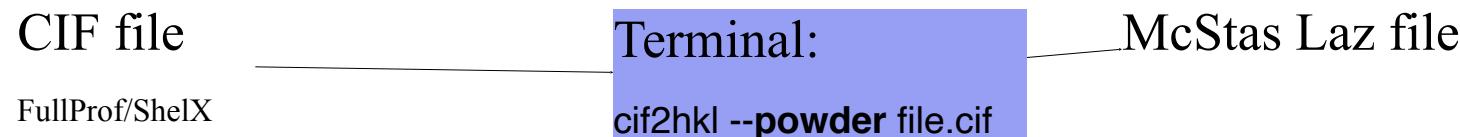
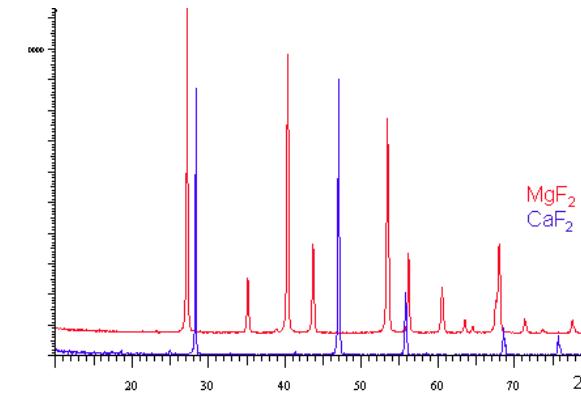


- | \$MCSTAS/data
 - | Windows: c:\mcstas-2.5\lib\data
 - | Linux: /usr/(local)/share/mcstas/2.5/data
 - | OS X: /Applications/McStas-2.5/Contents/Resources/mcstas/2.5/data
- | - Or make your own via
 - | Finding a CIF file for the given structure
 - | e.g. from ICSD <http://icsd.fiz-karlsruhe.de> or 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 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)



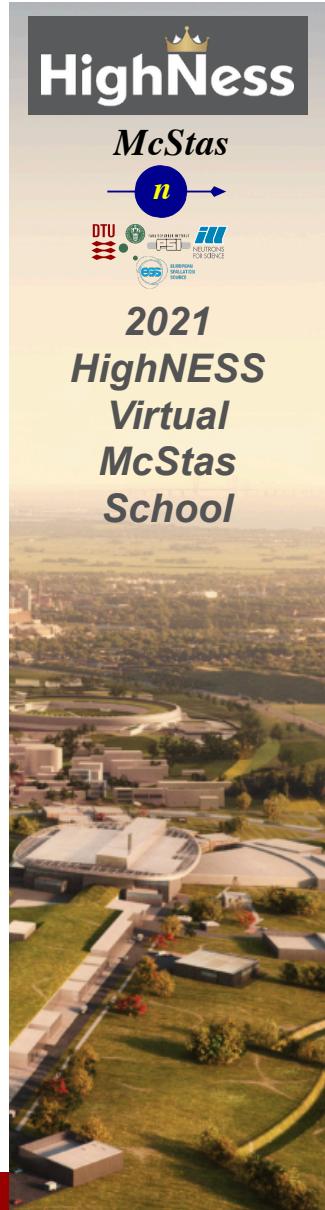
OFF/PLY any geometry



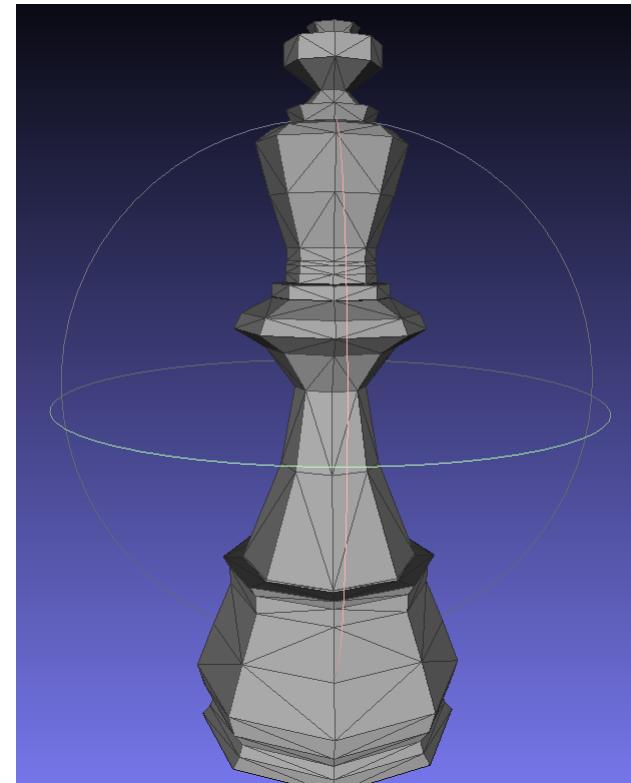
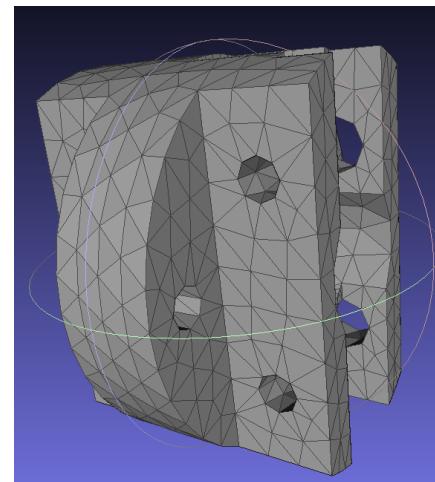
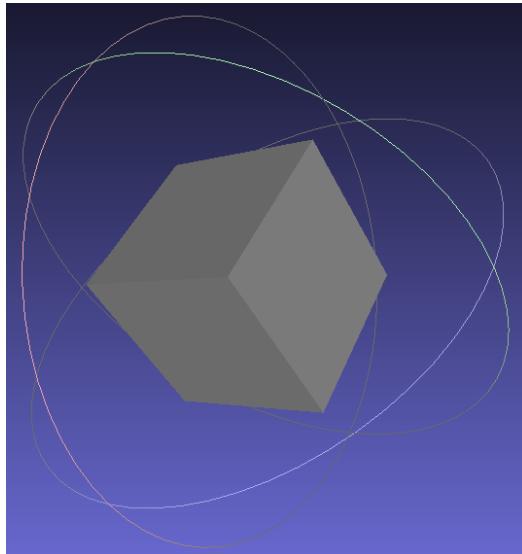
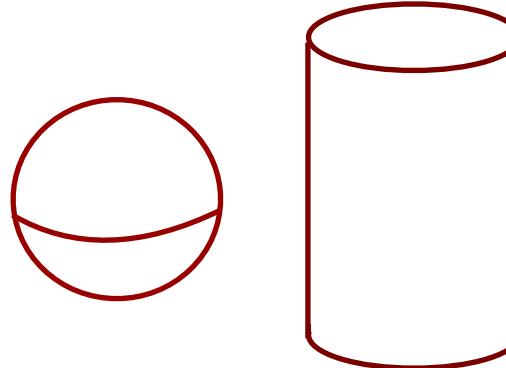
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An additional complex geometry enables to use any point set to describe the material volume (geomview OFF file).



HighNess

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