# SAMPLES
## (incoherent)


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In this session:

- Very brief description on neutron interactions with samples
- Types of samples in McStas
- Presentation of Incoherent Scattering Samples available in McStas

**IMPORTANT:**

All (and more) of this information can be found in the online pdf component documentation
http://www.mcstas.org/documentation/manual/mcstas-2.2a-components.pdf

also distributed with your McStas installation

The component documentation along with the "*mcdoc component_you_are_searching_for*" command, are your best friends when using McStas

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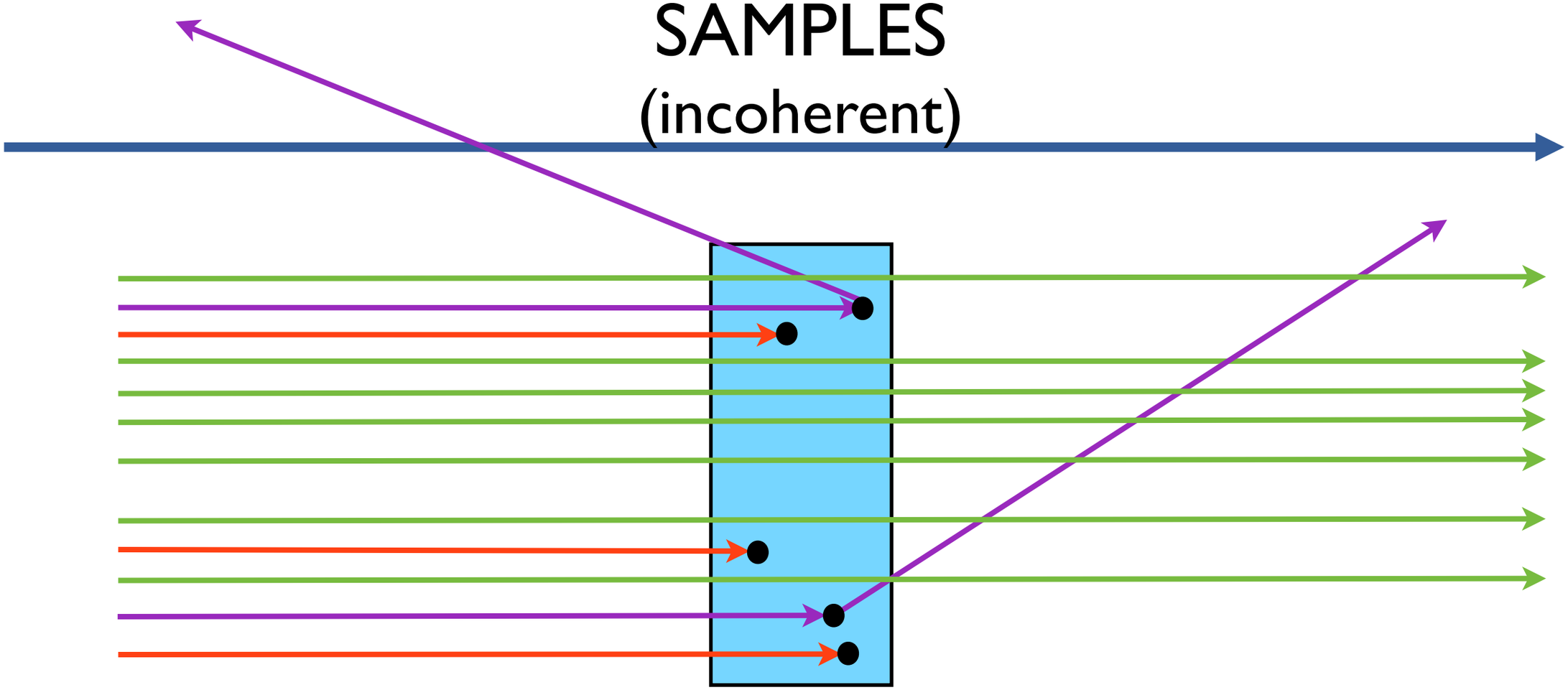
## (incoherent)



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

with probabilities: $p_A + p_T + p_S = 1$

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

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

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

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

**t =** sample thickness

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

macroscopic cross section [$cm^{-1}$]

number density [$atoms/cm^3$]

microscopic cross section [barn/atom]

1 barn = $10^{-24} cm^2$

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- High absorbing probability materials: **$^{3}$He, $^{6}$Li, $^{10}$B, $^{113}$Cd, $^{135}$Xe, $^{157}$Gd.**
- Neutron Scattering Cross Sections vary with atomic number but are not proportional to it (as is the case with X-rays).
- Scattered Neutrons:
  - Energy exchange with sample (inelastic scattering / spectroscopy experiments)
  - No energy exchange with sample (elastic scattering / diffraction experiments)
- Scattering can also be
  - Coherent
    - For most elements coherent scattering cross section is much higher than the incoherent
    - **Hydrogen** is an important exception, with **huge incoherent cross section**
  - Incoherent: no constructive interference between neutron waves scattered by different nuclei on the sample.
    - **Vanadium** has a **large incoherent cross section and almost no coherent cross section**. Widely used for instrument calibration and normalization

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- *V_sample.comp , Incoherent.comp:* Incoherent scattering (and absorption)
- *PowderN.comp :* Elastic Bragg scattering from an ideal powder ***[PW]***
- *Single_crystal.comp :* Bragg scattering from single crystals ***[PW]***
- *Isotropic_Sqw.comp :* General sample for isotropic materials
  *(coherent and incoherent, elastic and inelastic, with absorption and multiple scattering)* ***[EF]***
- Small ANgle Scattering **[CK]**

# SAMPLES
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Sample components in McStas

| Sample Process | Coherent Elastic | Coherent Inelastic | Incoherent Elastic | Incoherent Inelastic | Absorption | Multi. Scatt. |
|---|---|---|---|---|---|---|
| Phonon_simple | | X | | | 1 | |
| Isotropic_Sqw | X | X | X | X | 2 | X |
| Powder1 | 1 line | | X | | 1 | |
| PowderN | N lines | | X | | 1 | |
| Sans_spheres | colloid | | | | 1 | |
| Single_crystal | X | | X | | 2 | X |
| V_sample | | | X | QE broad. | 1 | |
| Tunneling_sample | | X | X | QE broad. | 1 | |

Table 8.1.: Processes implemented in sample components. Absorption: 1=single only, 2=with secondary

**Updated Table of McStas Samples follows**

# McStas sample model functionality-matrix

Status of the McStas sample components, september 2015 (post McStas 2.2a / pre McStas 2.3)

See also: McStas sample models for Diffraction, McStas sample models for Imaging, McStas sample models for Large-scale Structures, McStas sample models for Spectroscopy

| | **McStas sample comp + author info in italic** | **Model description** | **Main use areas** | **Incoherent scattering** | **Absorption** | **Bragg or other elastic scattering (type)** | **Inelastic scattering (type)** | **Multiple scattering** | **Non-trivial sample geometry** |
|---|---|---|---|---|---|---|---|---|---|
| 1 | Incoherent (Vanadium, Plexiglass etc.) *McStas team* | Simple incoherent scatterer | Generic, imaging | ✓ | ✓ | ✗ | ✗ | ✓ (analytic approach) | ✓ |
| 2 | Tunelling_sample *McStas team / Kim Lefmann* | Idem 1, plus tunneling peaks and QE broadening | Quasi-elastic scattering, backscattering | ✓ | ✓ | ✗ | ✗/✓ (Quasielastic broadening) | ✓ (analytic approach) | ✓ |
| 3 | PowderN *McStas team / Peter Willendrup* | Debye-scherrer cones, tabular input (lau / laz) | Powder diffraction, imaging | ✓ | ✓ | ✓ (Debye-Scherrer cones) | ✗ | ✗ | ✓ |
| 4 | Sample_nxs *Mirko Boin, HZB* | Debye-scherrer cones, unit-cell / atom input list | Powder diffraction, (future: imaging) | ✓ | ✓ | ✓ (Debye-Scherrer cones) | ✗/✓ | ✓ | ✗ |
| 5 | Single_crystal *McStas team* | Bragg spots, tabular input (lau). "Perfect imperfect" single crystal with mosaicity / lattice variation | Single crystal and MX diffraction | ✓ | ✓ | ✓ (Bragg spots) | ✗ | ✓ | ✓ |
| 6 | Sans_spheres (and other similar) *McStas team and Martin Cramer Pedersen, KU* | Hard spheres in thin solution and other models, defined per-component... | SANS | ✓ | ✓ | "✓" - SANS | ✗ | ✗ | ✗ |
| 7 | SANS_benchmark2 (and a few other stand-alone models) *Heinrich Frielinghaus, FZJ/JCNS* | Experimentally-benchmarked model set for SANS | SANS | ✓ | ✓ | "✓" - SANS | ✗ | ✓ up to 10 orders | ✗ |
| 8 | SASview_models !yet **unreleased**! *McStas team* | "Any" model from SASview / SASmodels | SANS | ✓ | ✓ | "✓" - SANS | ✗ | ✗ at this point | ✗ |
| 9 | Multilayer_sample *Rob Dalgliesh, ISIS STFC* | Multilayer-sample (dynamic scattering theory) with incoherent background | Reflectometry | ✓ | ✓ | "✓" - Reflectivity curve | ✗ | ✗ | ✗ |
| 10 | Phonon_simple *McStas team / Kim Lefmann* | Single-branch acoustic phonon in FCC lattice | Inelastic scattering phonons | ✗ | ✗ | ✗ | ✓ (phonon, at this point FCC lattice only) | ✗ | ✗ |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 11 | Isotropic_Sqw<br><br>*McStas team / Emmanuel Farhi* | Structure and dynamics<br><br>in isotropic materials<br><br>(liquids, powders etc.) | Inelastic scattering, diffraction,<br><br>isotropic materials, imaging | ✅ | ✅ | ✅ (Debye-<br><br>Scherrer cones) | ✅ isotropic inelastic<br><br>scattering | ✅ | ✅ |
| 12 | Res_sample<br>*McStas team* | Resolution-oriented<br><br>sample component | Generic | "✅" | ❌ | ❌ | "✅" flat, isotropic inelastic<br><br>scattering | ❌ | ❌ |
| 13 | TOFRes_sample<br>*McStas team / Kim Lefmann* | Idem Res_sample, with TOF<br><br>support | Generic | "✅" | ❌ | ❌ | "✅" flat, isotropic inelastic<br><br>scattering | ❌ | ❌ |
| 14 | Spot_sample<br><br>*Garrett Granroth, SNS/ORNL* | Resolution-oriented<br><br>sample component<br><br>Dirac delta-functions in (Q and energy) | Inelastic scattering | ❌ | ❌ | "✅" | "✅" | ❌ | ❌ |
| 15 | **Below this line not yet<br><br>available in repo** | **Below this line not yet<br><br>available in repo** | **Below this line not yet<br><br>available in repo** | **Below this line not yet<br><br>available in repo** | **Below this line not yet<br><br>available in repo** | **Below this line not yet<br><br>available in repo** | **Below this line not yet<br><br>available in repo** | **Below this line not yet<br><br>available in repo** | **Below this line not yet<br><br>available in repo** |
| 16 | "4D S(\vec(Q),\omega)"<br><br>Duc Le - soon at ISIS STFC? | Ala Isotropic_Sqw, but with crystal lattice | Elastic and inelastic<br><br>experiments with<br><br>crystals | ✅ | ✅ | ✅ | ✅ | ✅ | ?¿? |
| 17 | "Polycrystal"<br><br>*Alberto Cereser + Erik Knudsen, DTU Physics* | Engineering-diffraction / imaging oriented<br><br>multigrain sample | Engineering-diffraction / imaging | ✅ | ✅ | ✅ (Bragg spots) | ❌ | ✅ | ✅ |
| 18 | "Magnetic single crystal"<br><br>*Linda Udby KU, + Erik Knudsen, DTU* | Bragg spots from lattice ala Single_crystal<br><br>plus magnetic lattice. Tabular input (lau) | Single crystal magnetic diffraction | ✅ | ✅ | ✅ (Bragg spots) | ❌ | ✅ | ✅ / ?¿? |
| 19 | "Reflectometry sample"<br><br>*Jochen Stahn, PSI* | Reflectivity-curve sample | Reflectometry | ✅ | ✅ | "✅" - Reflectivity<br><br>curve | ❌ | ❌ | ❌ |

# SAMPLES
# (incoherent)

**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 |

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| Name | Unit | Description | Default |
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| 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 |
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| pack | 1 | Packing factor | 1 |
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| 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 |

**Examples:**

```
COMPONENT inc_sample = Incoherent(radius=0.05,focus_r=0.035, pack=1,
                                  target_index=1)
COMPONENT inc_sample = Incoherent(geometry="socket.off",focus_r=0.035,
                                  pack=1, target_index=1)
```

# SAMPLES
# (incoherent)

**V_sample.comp** An incoherent scatterer (cylindrical and spherical sample option )

[Rectangular shape also possible]

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

| Name | Unit | Description | Default |
|---|---|---|---|
| radius | m | Outer radius of sample in (x,z) plane | 0 |
| thickness | m | Thickness of outer wall | 0 |
| zdepth | m | depth of box sample | 0 |
| Vc | AA^3 | Unit cell volume | 13.827 |
| sigma_abs | barns | Absorbtion cross section pr. unit cell | 5.08 |
| sigma_inc | barns | Incoherent scattering cross section pr. unit cell | 5.08 |
| radius_i | m | radius-thickness | 0 |
| radius_o | m | Same as radius | 0 |
| h | m | Same as yheight | 0 |
| focus_r | m | Radius of disk containing target. Use 0 for full space | 0 |
| pack | 1 | Packing factor | 1 |
| frac | 1 | MC Probability for scattering the ray; otherwise penetrate | 1 |
| f_QE | 1 | Fraction of quasielastic scattering (rest is elastic) | 0 |
| gamma | 1 | Lorentzian width of quasielastic broadening (HWHM) | 0 |
| target_x | - | | 0 |
| target_y | m | position of target to focus at | 0 |
| target_z | - | | 0 |
| focus_xw | m | horiz. dimension of a rectangular area | 0 |
| focus_yh | m | vert. dimension of a rectangular area | 0 |
| focus_aw | deg | angular width dimension of a rectangular area | 0 |
| focus_ah | deg | angular height dimension of a rectangular area | 0 |
| xwidth | m | horiz. dimension of sample | 0 |
| yheight | m | vert. dimension of sample | 0 |
| zthick | m | Same as zdepth | 0 |
| rad_sphere | m | Radius for a spherical sample | 0 |
| sig_a | barns | Same as sigma_abs | 0 |
| sig_i | barns | Same as sigma_inc | 0 |
| V0 | AA^3 | Same as Vc | 0 |
| target_index | 1 | relative index of component to focus at, e.g. next is +1 | 0 |
| multiples | 1 | Apply crude estimate for multiple scattering | 1 |

# SAMPLES
# (incoherent)

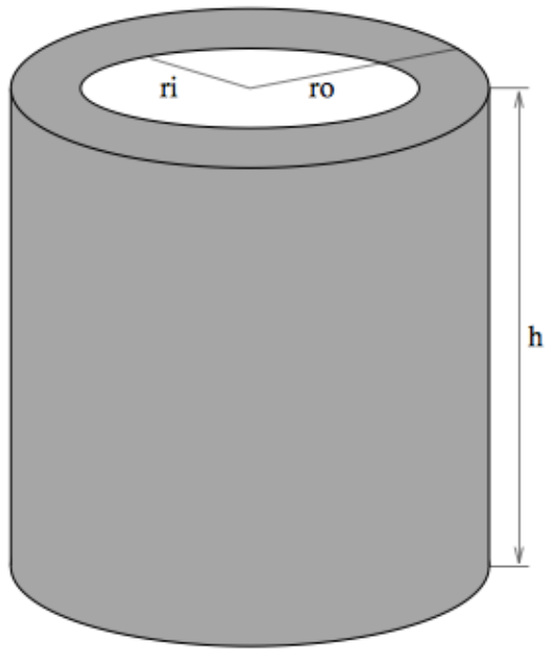
## V_sample.comp

An incoherent scatterer (cylindrical and spherical sample option)

[Rectangular shape also possible]

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

| Name | Unit | Description | Default |
|---|---|---|---|
| radius | m | Outer radius of sample in (x,z) plane | 0 |
| thickness | m | Thickness of outer wall | 0 |
| zdepth | m | depth of box sample | 0 |
| Vc | AA^3 | Unit cell volume | 13.827 |
| sigma_abs | barns | Absorbtion cross section pr. unit cell | 5.08 |
| sigma_inc | barns | Incoherent scattering cross section pr. unit cell | 5.08 |
| radius_i | m | radius-thickness | 0 |
| radius_o | m | Same as radius | 0 |
| h | m | Same as yheight | 0 |
| focus_r | m | Radius of disk containing target. Use 0 for full space | 0 |
| pack | 1 | Packing factor | 1 |
| frac | 1 | MC Probability for scattering the ray; otherwise penetrate | 1 |
| f_QE | 1 | Fraction of quasielastic scattering (rest is elastic) | 0 |
| gamma | 1 | Lorentzian width of quasielastic broadening (HWHM) | 0 |
| target_x | - | | 0 |
| target_y | m | position of target to focus at | 0 |
| target_z | - | | 0 |
| focus_xw | m | horiz. dimension of a rectangular area | 0 |
| focus_yh | m | vert. dimension of a rectangular area | 0 |
| focus_aw | deg | angular width dimension of a rectangular area | 0 |
| focus_ah | deg | angular height dimension of a rectangular area | 0 |
| xwidth | m | horiz. dimension of sample | 0 |
| yheight | m | vert. dimension of sample | 0 |
| zthick | m | Same as zdepth | 0 |
| rad_sphere | m | Radius for a spherical sample | 0 |
| sig_a | barns | Same as sigma_abs | 0 |
| sig_i | barns | Same as sigma_inc | 0 |
| V0 | AA^3 | Same as Vc | 0 |
| target_index | 1 | relative index of component to focus at, e.g. next is +1 | 0 |
| multiples | 1 | Apply crude estimate for multiple scattering | 1 |




**Example:**

```
COMPONENT van_sample = V_sample(radius_i=0.001,radius_o=0.01,h=0.02,
                                focus_r=0.035, pack=1, target_index=1)
```

# SAMPLES
# (incoherent)

## EXERCISE

- Open the existing instrument file named *'Samples_vanadium.instr'* (you will find it under *neutron site* --> *Tests_samples* at your mcgui window)

- Before running the instrument file, spend some time reading it and understanding what components it contains

    - The vanadium sample, as an incoherent scatterer should give a uniform angular distribution of scattered neutrons.
    - Run the *Samples_vanadium.instr* file as is, with 1e6 events. Do you get a uniform angular distribution? (shocking answer: NO!). Why is that?
    - Experiment with the thickness, the radius, and the pack factor of the *V_sample* component in the instrument file. What does the results you get tell you about the reason of the previously seen non-uniform distribution?