SAMPLES
(incoherent)

ESS McStas Training 2016
May 30th - June 1st

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<u>In this session:</u>

- 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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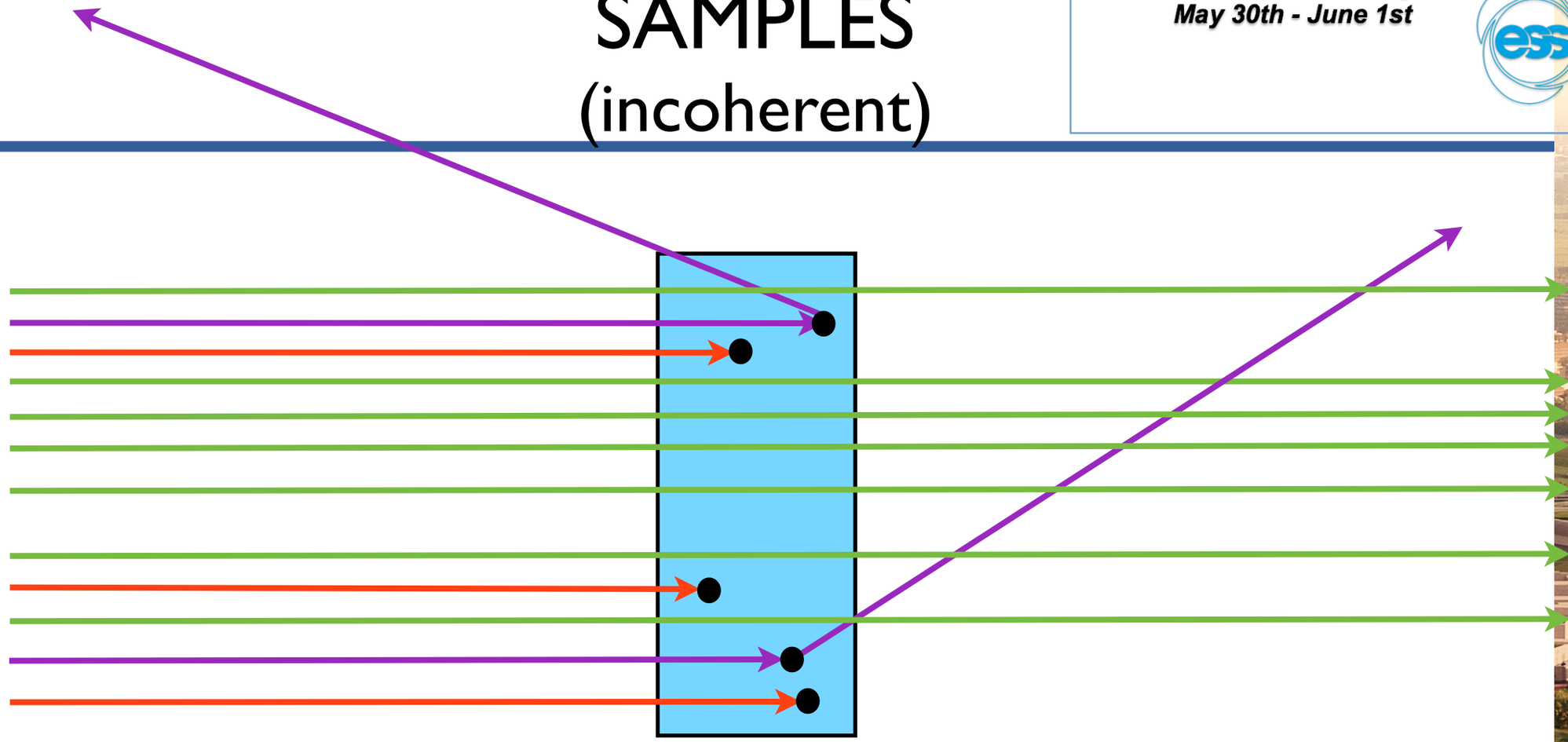
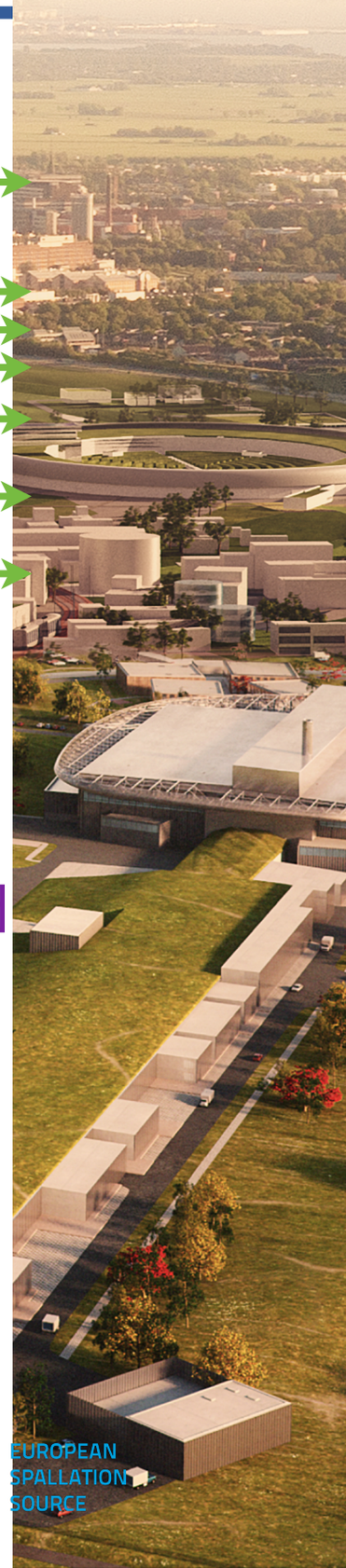


A neutron hitting a sample can be absorbed, transmitted, or scattered

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]

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Sample components in McStas

Sample	Coherent		Incoherent			
Process	Elastic	Inelastic	Elastic	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

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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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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)
```

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[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

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V_sample.comp

An incoherent scatterer (cylindrical and spherical sample option)

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

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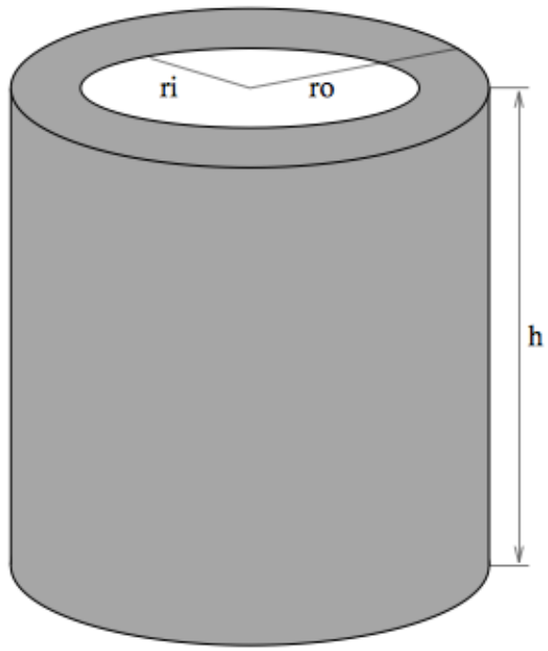
h	m	Same as yheight	0
focus_r	m	Radius of disk containing target. Use 0 for full space	0
pack	1	Packing factor	1
frac	1	MC Probability for scattering the ray; otherwise penetrate	1
f_QE	1	Fraction of quasielastic scattering (rest is elastic)	0
gamma	1	Lorentzian width of quasielastic broadening (HWHM)	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)
```

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EXERCISE