

Thursday



Diffraction

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You will now simulate both

- | *Exercise 5.2 on powders*
- | *Exercise 5.3 on single crystals*



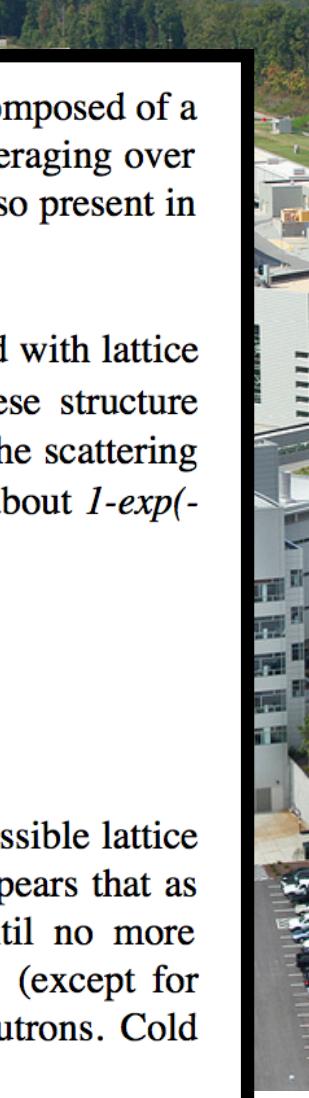
5.2 PowderN - intro

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.



5.2 PowderN - construct a simple instrument file

Construct the below instrument file using mcgui....

```
*****
* Instrument: powder_simple.instr
* %Description
* A powder scattering example.
*
* %Parameters
* lambda: [Angs] incoming neutron wavelength (monochromatic)
* material: [Angs] Powder structure file (lazy/fullprof/crystallographica)
*****
```

```
DEFINE INSTRUMENT powder_simple (Lambda=2.36, string material="Na2Ca3Al2F14.laz")
TRACE
```

```
COMPONENT Source= Source_simple(dist=1, radius=0.01, focus_xw=0.01, focus_yh=0.01, lambda0=Lambda,
dlambda=Lambda*0.01)
```

```
AT (0,0,0) ABSOLUTE
```

```
COMPONENT powder= PowderN(reflections = material, radius = 0.005, yheight = 0.05)
```

```
AT (0,0,0.5) RELATIVE PREVIOUS
```

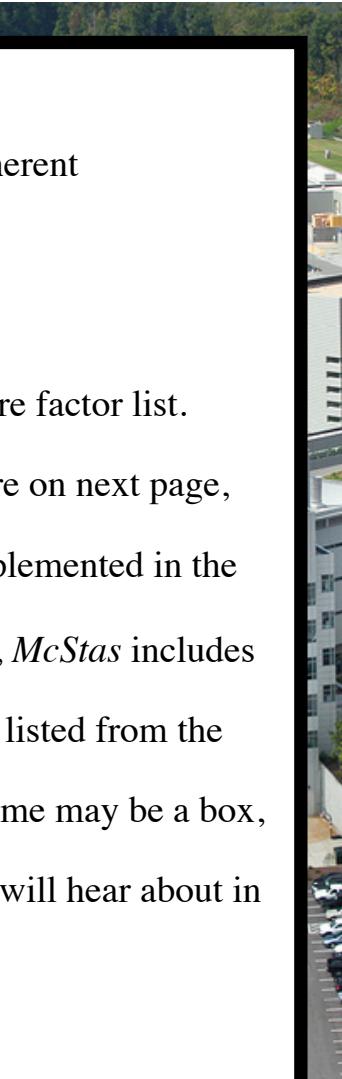
```
COMPONENT banana= Monitor_nD(xwidth=1, yheight=0.3, options="banana ; theta limits=[10,130] bins=240 ; y bins=50")
```

```
AT (0,0,0) RELATIVE PREVIOUS
```

```
END
```



5.2 - PowderN and datafiles



The equations from *Squires* relating to powders have been directly implemented in the ***PowderN*** component.

This handles single, coherent scattering and many d -spacing structure factors, with absorption correction and incoherent elastic scattering. However, no multiple or inelastic scattering is taken into account, which the *Isotropic_Sqw* component can cope with, in its powder mode (see exercise 9.4).

In the example at hand, we present a usage example which produces so-called Debye-Scherrer rings from a structure factor list. The model geometry is shown in the *left* figure on next page, and the 2D ideal diffraction detector in the *right* figure on next page, for a Na₂Ca₃Al₂F₁₄ reference powder. The choice of the material may be any file adapted from *Lazy/Pulverix* implemented in the ICSD database and *Fullprof* (extension *.laz*) or *Crystallographica* (extension *.lau* also used for crystals). Currently, *McStas* includes a material data base of about 70 powder and crystal definitions commonly used in neutron scattering. These can be listed from the *McGUI/Help/Component Library Index* menu item, and you may easily add your own materials. The material volume may be a box, a sphere and a cylinder, which all can be bulk or hollow geometries, including concentric arrangements, which we will hear about in exercise 11.

5.2 Perform simulations

Please run your newly created instrument file in trace mode and simulation mode to see output like the ones below.

Investigate how the peak positions change with varied wavelength, try $\pm 1 \text{ \AA}$ in wavelength.

Also try choosing another material from your MCSTAS/data directory.

As a final optional PowderN exercise, try studying the effect of sample size

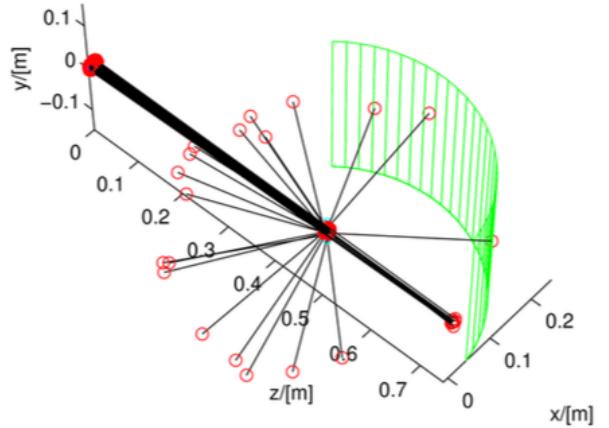


Figure 12a. Geometry of the *Example 8* simple powder diffraction setup, showing a few diffracted neutron trajectories. The beam is attenuated and scattered in the sample.

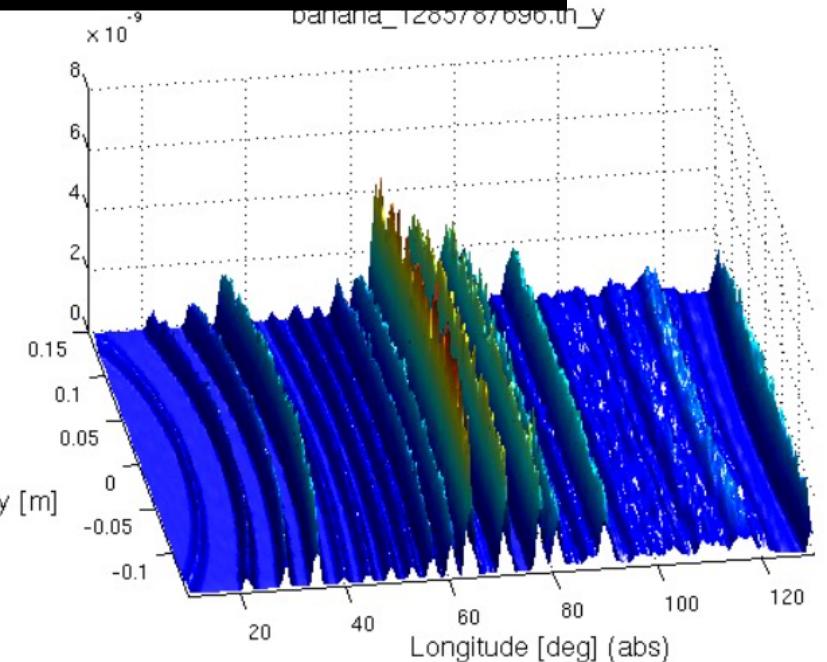


Figure 12b. Diffraction pattern obtained from a $\text{Na}_2\text{Ca}_3\text{Al}_2\text{F}_{14}$ powder at $\lambda=2.36 \text{ \AA}$, showing intensity vs. horizontal angle vs. vertical position along the detector.

5.3 Single_crystal - intro

When the sample is a single crystal, the averaging on many crystallites that is responsible for the scattering rings in a powder does not apply.

The Bragg law is still valid, but similarly as a mirror, each atomic plane selects a single reflected monochromatic ray. As there are many structural planes available, a polychromatic neutron beam will be scattered as a large number of distinct rays, forming spots on detectors.

This happens in the monochromators as discussed during the session on optics, but in this case only one reflection of interest is used, the others are scattered around, generating background.



5.3 Single_crystal - construct a simple instrument file

Construct the below instrument file using mcgui....

```
*****
* Instrument: single_crystal.instr
* %Description
* A single crystal scattering example.

*
* %Parameters
* lambda: [Angs] neutron wavelength selected by the monochromator
*****
```

DEFINE INSTRUMENT single_crystal (*Lambda*=1, string *material*="C_graphite.lau")

TRACE
 COMPONENT Source= Source_simple(dist=1, radius=0.01, focus_xw=0.01, focus_yh=0.01, lambda0=*Lambda* dlambda=0.2**Lambda*),

AT (0,0,0) ABSOLUTE

COMPONENT SX = Single_crystal(
 xwidth = 0.002, yheight = 0.1, zdepth = 0.1, mosaic = 30, reflections = *material*, barns=0, ax=0, ay=2.14,az=1.24,
 bx=0, by=0, bz= 2.47, cx=6.71,cy=0, cz= 0, absorption = 0.014, incoherent = 0.004)

AT (0,0,0.5) RELATIVE PREVIOUS

ROTATED (0,45,0) RELATIVE PREVIOUS

COMPONENT banana= Monitor_nD(xwidth=1, yheight=1, options="banana ; theta limits=[10,130] bins=240 ; y bins=100")

AT (0,0,0.5) RELATIVE Source

END



5.3 Single_crystal input parameters



The **Single_crystal** component is used the same way as the PowderN, but only accepts .lau type files from e.g. Crystallographica.

This component models coherent and incoherent elastic scattering, with multiple scattering and secondary absorption.

The material volume may be a box, a sphere and a cylinder, which all can be bulk or hollow geometries, including concentric arrangements.

The instrument geometry resembles the previous one for PowderN, now with a tilted graphite plate at the sample. As expected, the scattering shows a number of spots, which each select a single wavelength. The central spot is the direct, transmitted beam.

Currently, McStas does not provide simple ways to add inelastic scattering on top of a mono-crystalline structure, even though there is a way to simulate the neutron scattering on a simple phonon dispersion.

Perform simulations

- Now perform trace to see that all looks OK, then a simulation that should give you output like this:

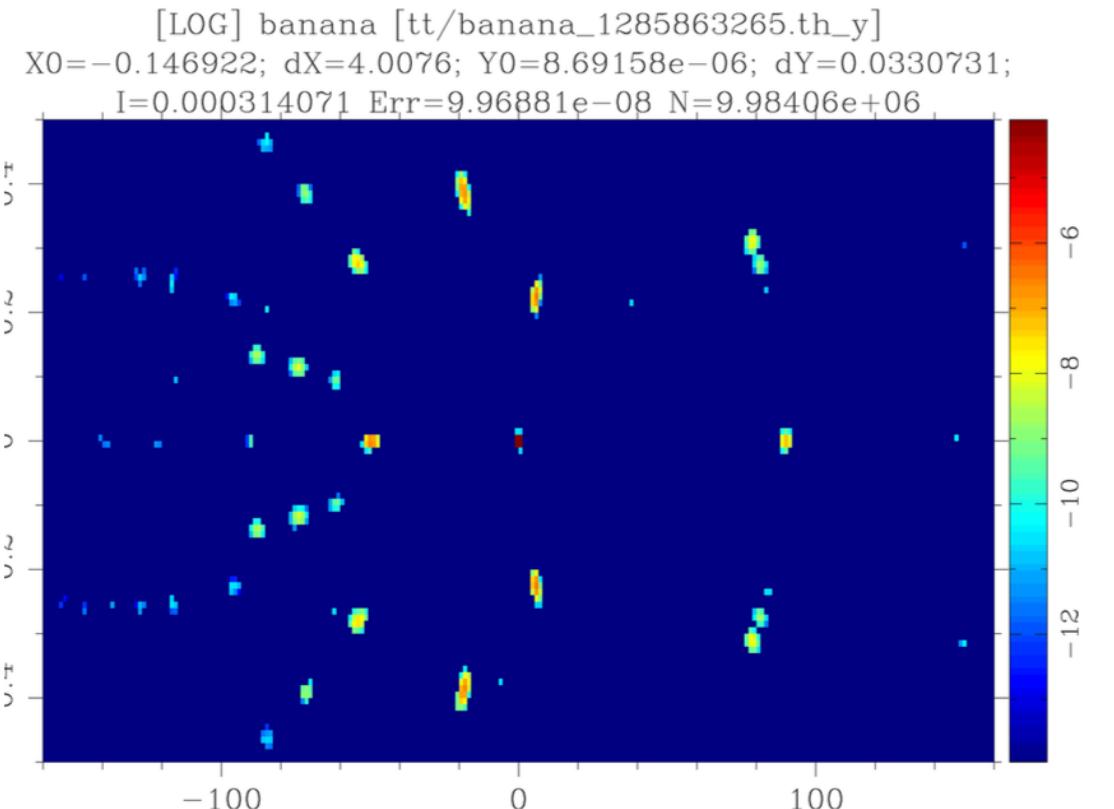
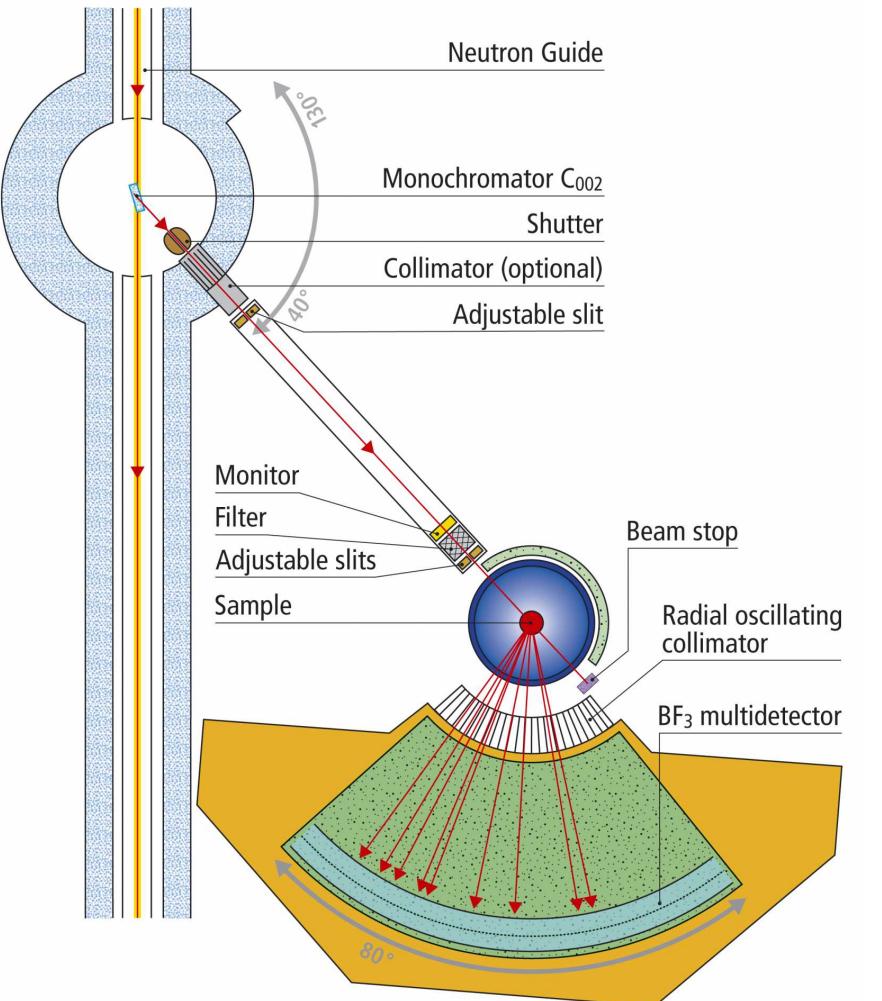


Figure 14. Neutron scattering from a single crystal of graphite from a neutron beam around $\lambda=1 \text{ \AA}$, obtained from the *Example 10*. Intensity is shown as a function of the horizontal angle and vertical coordinate, in log scale, with colors ranging from blue (low) to red (high).



Real Instruments

PSI DMC



File → New from Template
→ PSI_DMC

Run the instrument with it's default parameters.

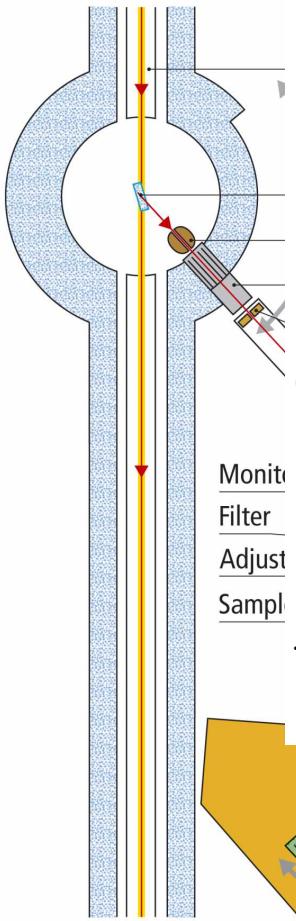
Now we'll try to insert a Single crystal instead of the default Powder.



Real Instruments

PSI DMC

Increase the height of the detector and make it resolve the signal along y.



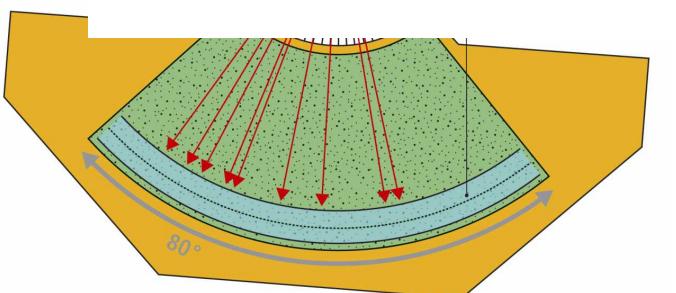
Set:

Options="banana, theta y auto limits bins=20", yheight=0.3

In the detector.

...and change the sample to be e.g. an Aluminium crystal.

```
COMPONENT single_crystal = Single_crystal(
    reflections="Al.lau",
    yheight=0.05, radius=0.01, mosaic=1, delta_d_d=1e-4,
    az=4.0495, ay=0, ax=0, bx=4.0495, by=0, bz=0,
    cx=0, cy=4.0495, cz=0,
    p_transmit=0.1)
AT (0, 0, 0) RELATIVE PREVIOUS
```



TOPAZ and SENJU

Take a look at a couple of “real” instrument simulations of Laue Cameras: they both resides in the Dropbox under
 “McStas_Diffract, Laue”

1. SNS TOPAZ
2. J.PARC SENJU (aka. BL18)

Here you need to also copy a datafile for the J-PARC source
“source_BL18.txt”

Surgeon General's Warning:
 There are lots of COMPONENTS here



Optional extras

- | Create an *instrument input parameter omega* to allow rotating the sample.
- | Perform a scan and look in the subfolders how the spots move on the detector.
- | Also try
 - Decreasing and increasing the wavelength spread
 - Comment on the results



Optional extras



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

Try the same simulations with an OFF file from the MCSTAS/data directory