



# IDS for Diffraction

DREAM and MAGIC

CÉLINE DURNIK

# Agenda



- 1 Instruments
- 2 Status of data processing for DREAM
- 3 Project management
- 4 Communication
- 5 MAGIC
- 6 Other scientific projects
- 7 Future plans

# Overview

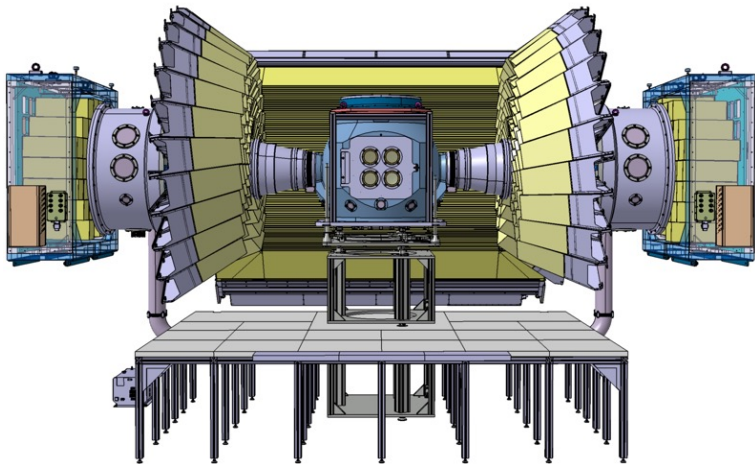
## Diffraction at ESS for DREAM and MAGIC

- **DREAM** bi-spectral powder diffractometer

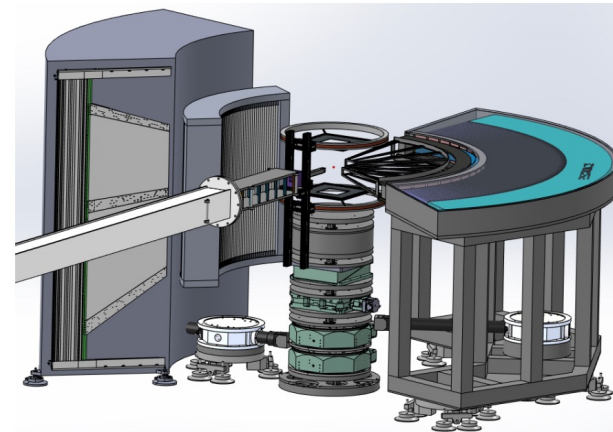
*Science cases:* Powder diffraction, Single crystal diffraction, PDF, SANS, polarized neutrons

- **MAGIC** polarized single-crystal diffractometer

*Science cases:* Single crystal diffraction, polarized neutrons, powder diffraction



*DREAM detector configuration (full coverage) and sample vessel*



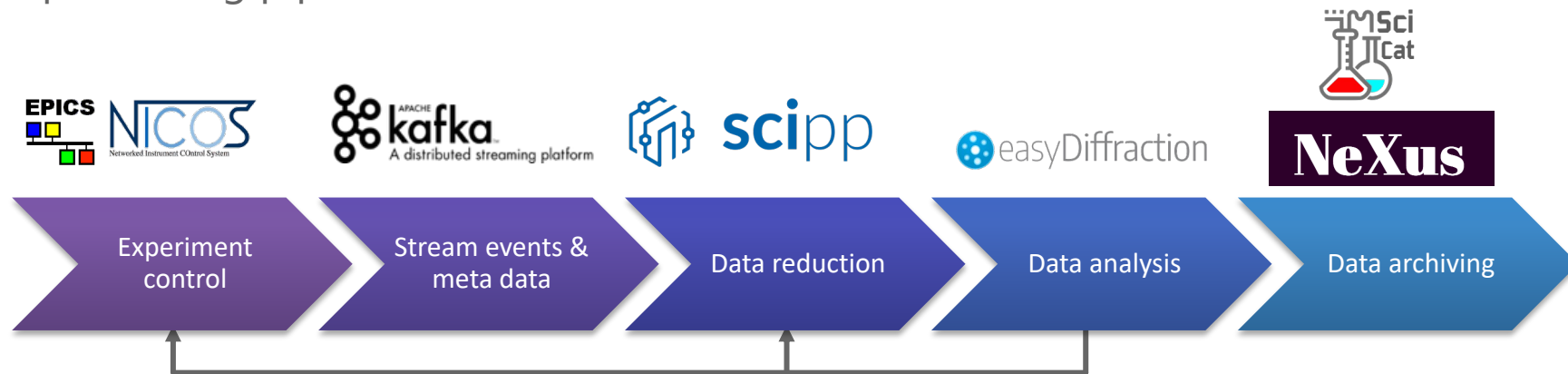
*MAGIC detector configuration*

- Development focused on DREAM, easily applied to MAGIC

# Overview

## Diffraction at ESS for DREAM and MAGIC

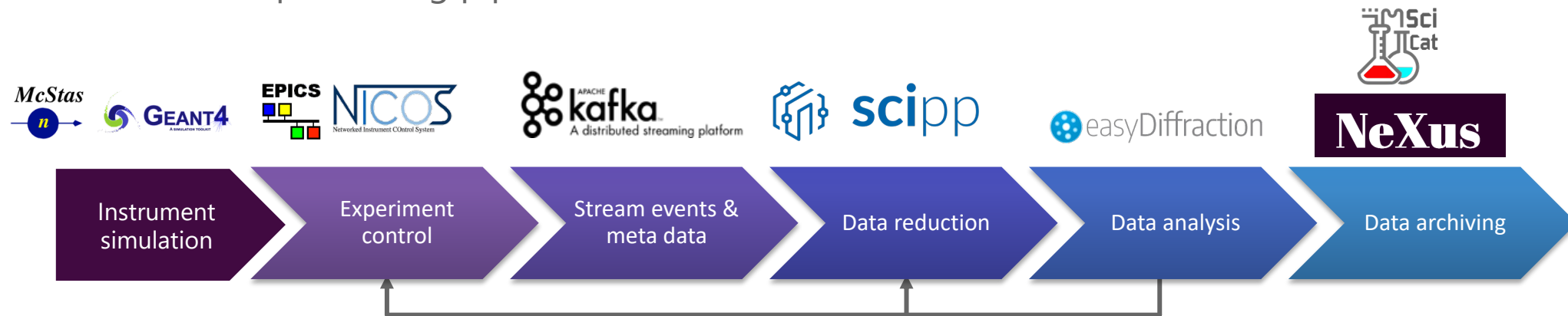
- Development focused on DREAM
- DMSC data processing pipeline



# Overview

## Diffraction at ESS for DREAM and MAGIC

- Development focused on DREAM
- DMSC data processing pipeline



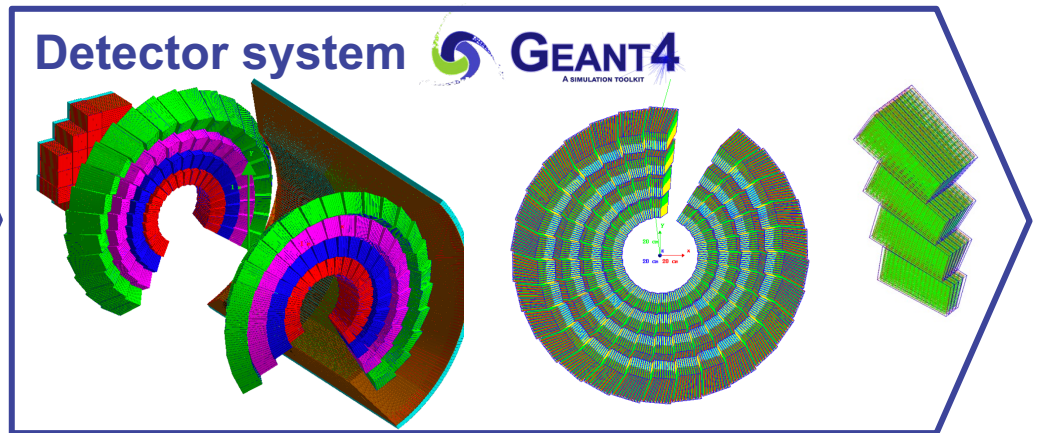
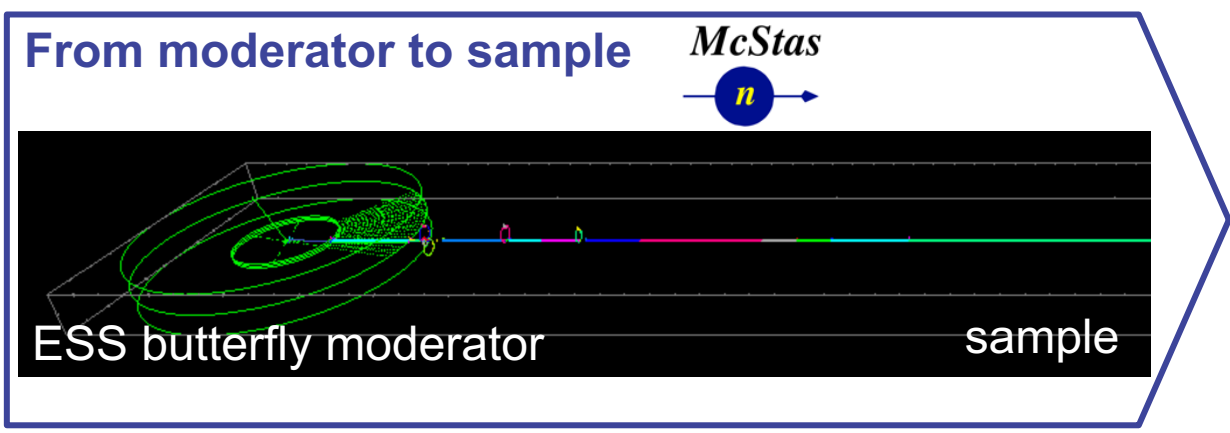
# Instrument simulation

## Instrument simulation

**McStas**  
 Monte Carlo ray-tracing simulation

**GEANT4** A SIMULATION TOOLKIT toolkit for simulating passage of particles through matter

## Method

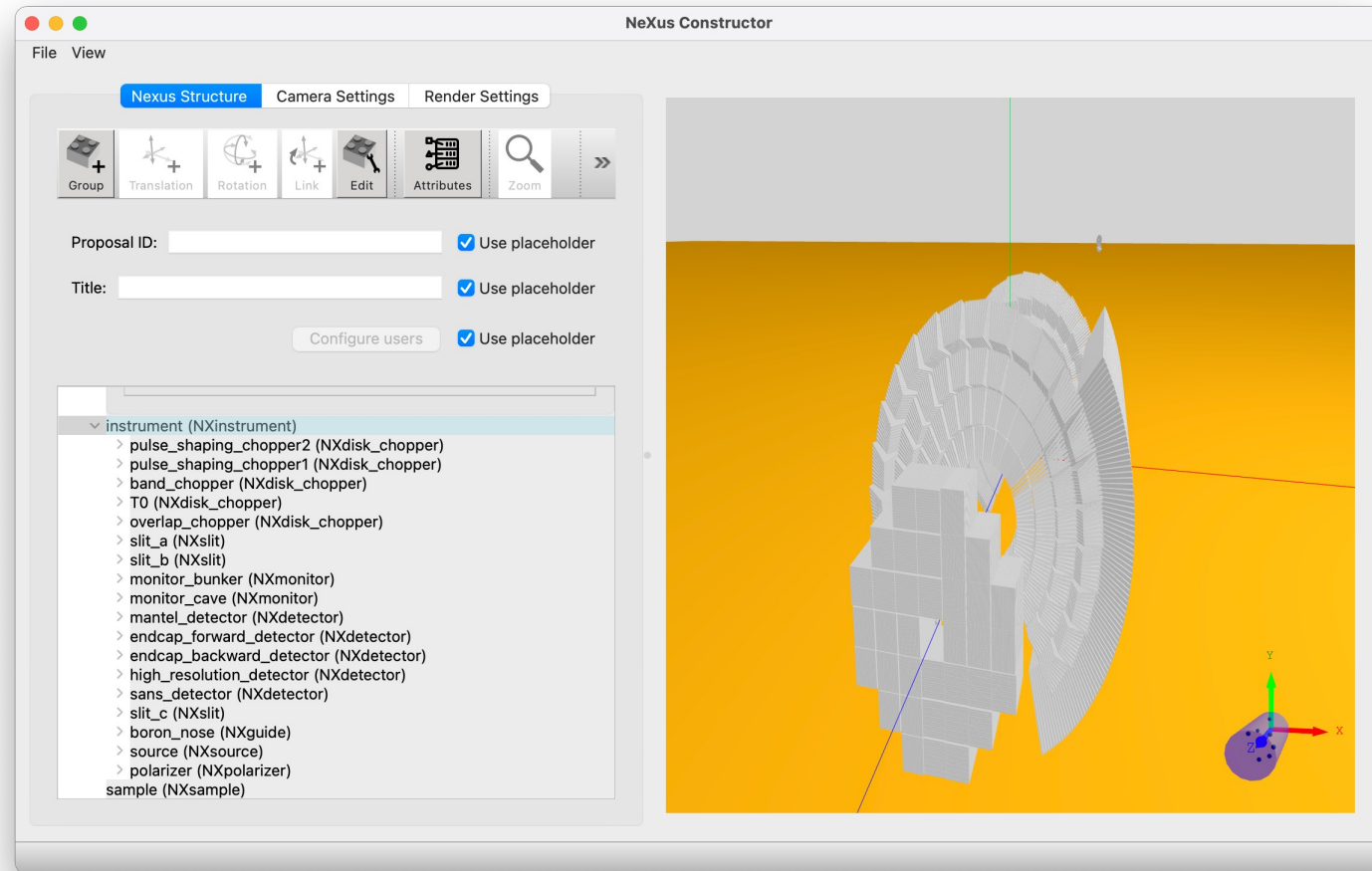


SANS detector not modelled in GEANT4 yet

# Data processing for DREAM

## NeXus files

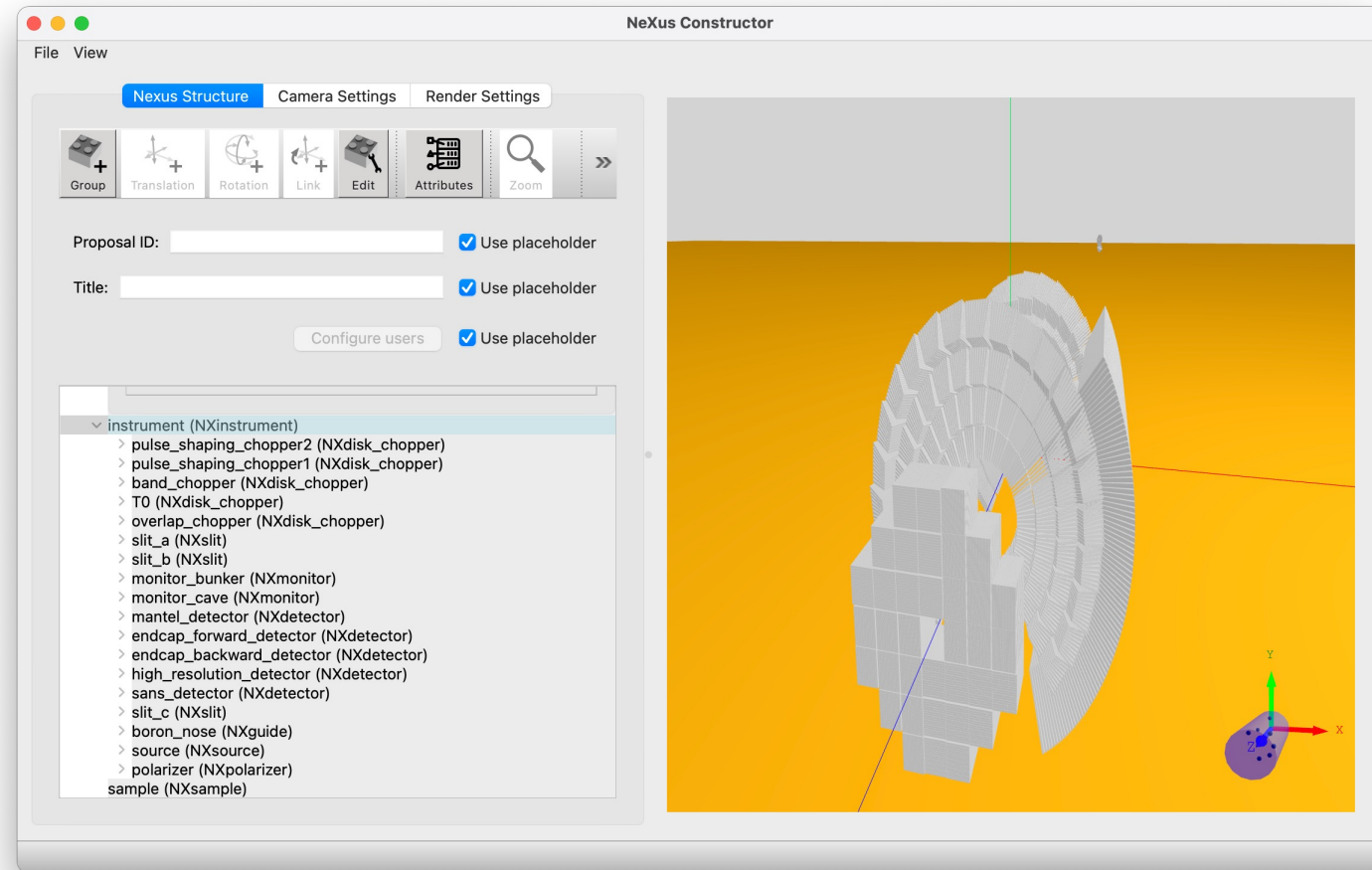
- Baseline developed by ECDC for DREAM
  - All components stored in files
  - No neutron events
  - No interface with McStas, GEANT4



# Data processing for DREAM

## NeXus files

- Baseline developed by ECDC for DREAM
  - All components stored in files
  - No neutron events
  - No interface with McStas, GEANT4



- **Temporary solution to develop the data processing pipeline:**  
csv file from GEANT4 as input to data reduction

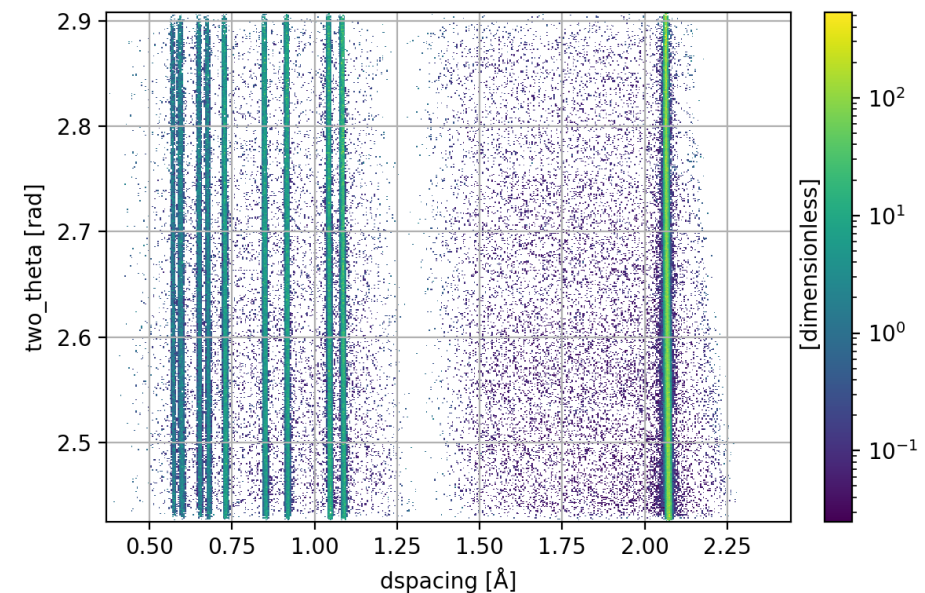
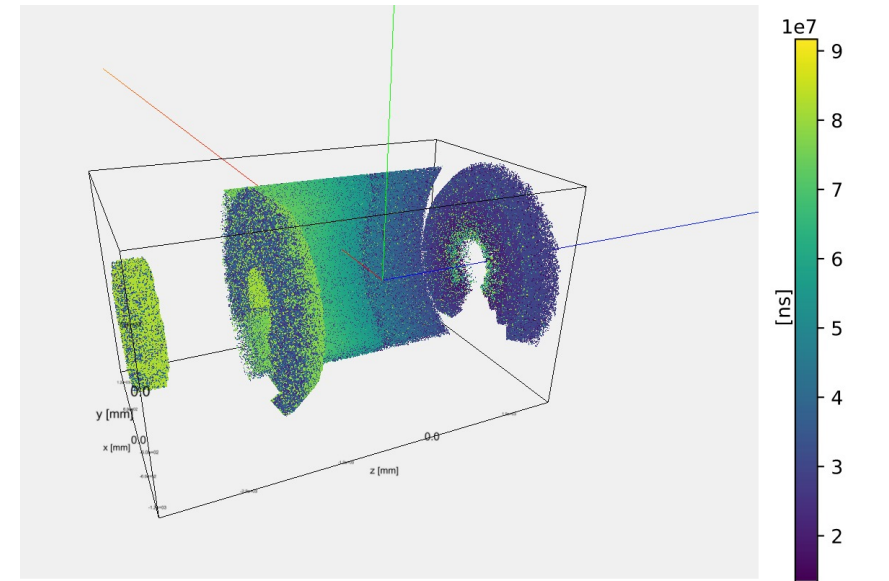


# Data processing for DREAM

Scipp: example of what can be done

**Input:** csv file using Diamond powder sample

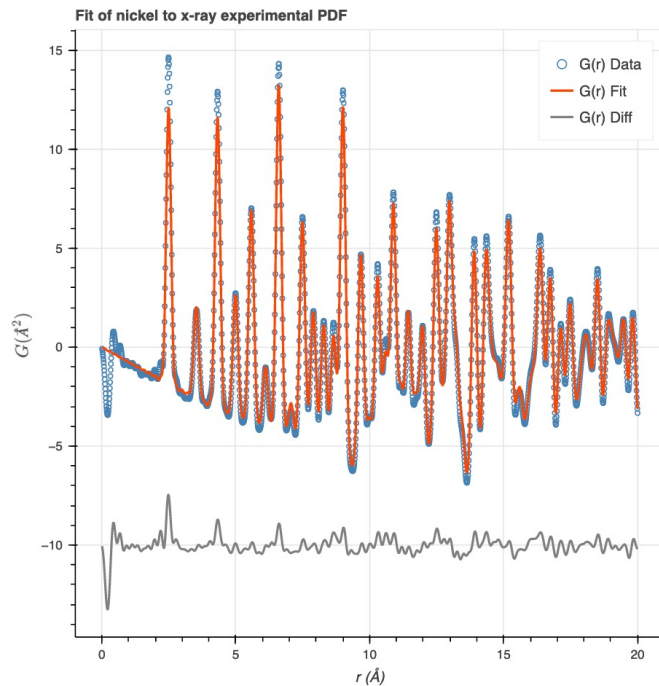
- select endcap backward detectors
- convert to d-spacing
- add  $2\theta$  coordinates
- normalize by Vanadium



# Data processing for DREAM

## Analysis

Recent development in EasyDiffraction:  
Support for Pair Distribution Function using PDFfit2



### Fit PDF profile

This notebook illustrates how to fit 1D PDF profile in EasyDiffraction for X-ray experimental data and Ni sample using PDFfit2 (J. Phys. Condens. Matter **19**, 335219 (2007). doi: <https://doi.org/10.1088/0953-8984/19/33/3352190>).

```
[1]: import os

from easyCore.Fitting.Fitting import Fitter
from easyDiffractionLib import Phases
from easyDiffractionLib.Jobs import Powder1DCW
from easyDiffractionLib.interface import InterfaceFactory as Calculator
from easyDiffractionLib.Profiles.P1D import PDFParameters
from easyDiffractionLib.Interfaces.pdfFit2 import readGRData

# for plotting
from bokeh.io import show, output_notebook
from bokeh.plotting import figure
output_notebook()
FIGURE_WIDTH = 900
FIGURE_HEIGHT = 300
```

Loading BokehJS ...

### Define calculator

```
[2]: calculator = Calculator()
calculator.switch("PdfFit2")
```

### Load experimental and reference data

`Ni-xray.gr` contains reduced X-ray data with Ni sample. Its structure is a header with metadata and then an array of 4 columns:  $r$ ,  $G(r)$ , and the error related to these 2 quantities. The reduction was done with `pdfgetx2`.

```
[3]: data_fname = os.path.realpath('Ni-xray.gr')
data = readGRData(data_fname)
cif_fname = os.path.realpath('Ni.cif')
phases = Phases.from_cif_file(cif_fname)
```

### Define job

```
[4]: parameters = PDFParameters()

[5]: job = Powder1DCW('Ni', parameters=parameters, phases=phases, interface=calculator)
fitter = Fitter(job, calculator.fit_func)
```



# Data processing for DREAM

## Analysis

### **Recent development in EasyDiffraction:**

Support for Pair Distribution Function using PDFFit2

### **Collaborations with**

- ILL on Python bindings of CrysFML
- Chalmers university for implementation of X-ray support in EasyDiffraction



# Project planning

## For DREAM

**Jira dashboard** for DSMC development for DREAM for **cold** and **hot** commissioning and **first science**

Tasks related to

User Office  
VISA  
Scicat

Scichat  
Instrument Control  
NeXus

Instrument Simulation  
Reduction  
Analysis



# Project planning

## For DREAM

**Jira dashboard** for DSMC development for DREAM for cold and hot commissioning and first science

Tasks related to

User Office  
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Instrument Control  
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**Milestones** = focus for the next 18 months

1. Post-beamtime data processing workflow ready for 1D Powder diffraction at DREAM
2. Post-beamtime data processing workflow for Pair Distribution Function at DREAM
3. Real-time data processing for 1D Powder diffraction for DREAM



# Communication

## Internal & external

- **Instrument teams**
  - Monthly meetings
  - Python trainings
  - Participation to beamtimes
- **ORNL**: meeting with instrument computer scientists (test data, experience...)
- **Conferences**
  - Journées de la diffusion neutronique 2022 (posters)
  - ECNS2023: talk and poster



# MAGIC

## Status

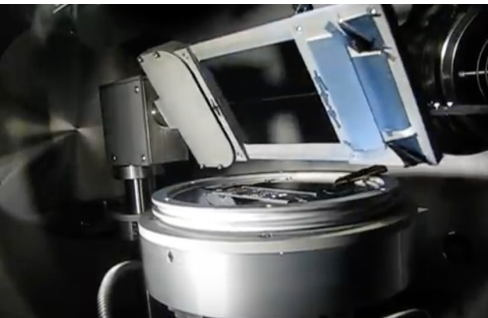
- **Instrument simulation:** modelling of detectors in GEANT4 in progress
- **Project management:** Requirements for data processing to be converted to JIRA dashboard
- Detector test at ISIS
- Quarterly meetings with instrument team

# Other projects

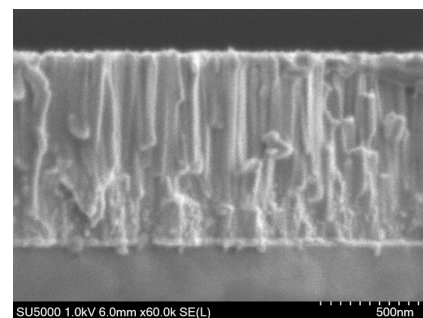
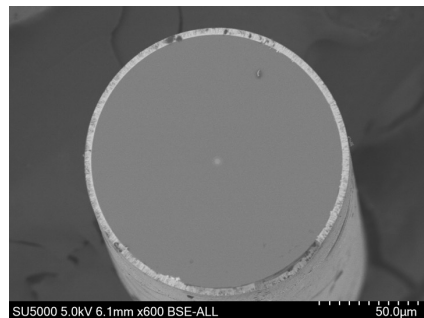
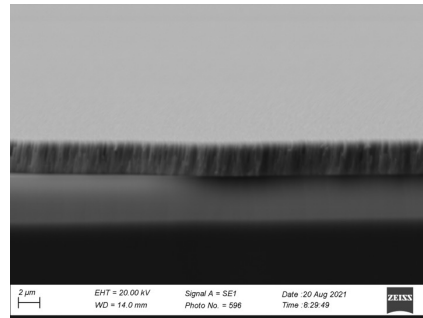
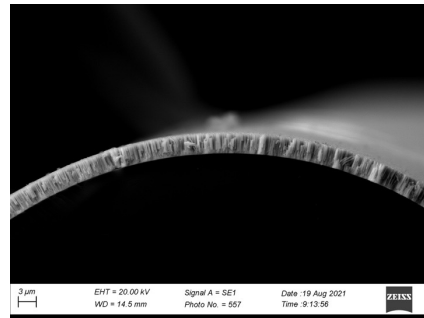
## Science and other scattering techniques

**Science:** collaboration with Defence Science and Technology Group, Adelaide Australia on magnetic thin films

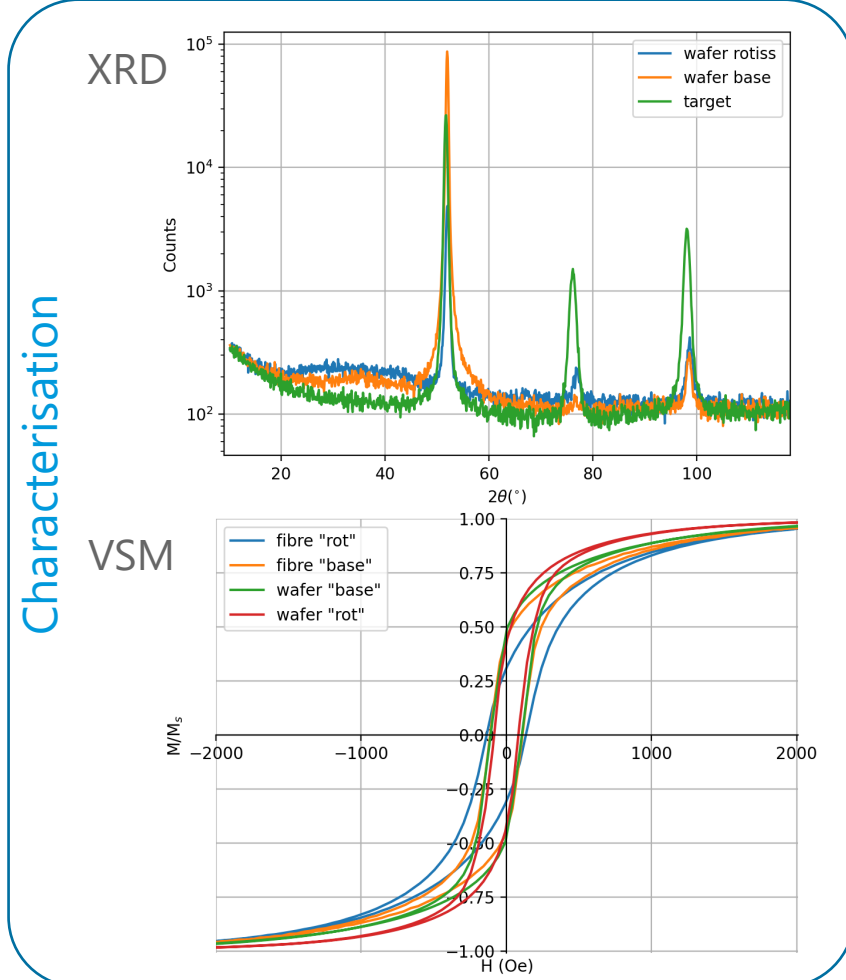
Film deposition



Deposition chamber



Examples of deposited thin films







# Other projects

## Science and other scattering techniques

**Science:** collaboration with Defence Science and Technology Group, Adelaide Australia on magnetic thin films

### Beamtimes

- DESY with Mikhail Feygenson (*science*)
- ILL commissioning (D10+)
- MAX IV with Mikhail Feygenson (*science*, May 2023)
- ISIS IMAT – 2<sup>nd</sup> test of DREAM bi-spectral switch (May 2023)

### QENS

- paper submitted to EPJ Web of conferences
- associated partner in ErUM-data project planning to use QENS library (*initially funded by SINE2020 Workpackage 10*)



# Plans

## Next 6 months

- **Delivery** related to **milestones**:
  - data & metadata added to ESS NeXus file
  - WFM and other reduction routines
  - interface reduction → analysis
  - instrument simulation and data reduction for Pair Distribution Function
  
- **Polarisation** for DREAM and MAGIC
  
- **Beamtimes** and related data processing
  
- **Paper** on magnetostrictive thin films
  
- IUCr2023 + **collaboration** in Australia



Thanks for your attention

Do you have any questions, comments?