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# MODI – a monochromatic powder diffractometer for ESS

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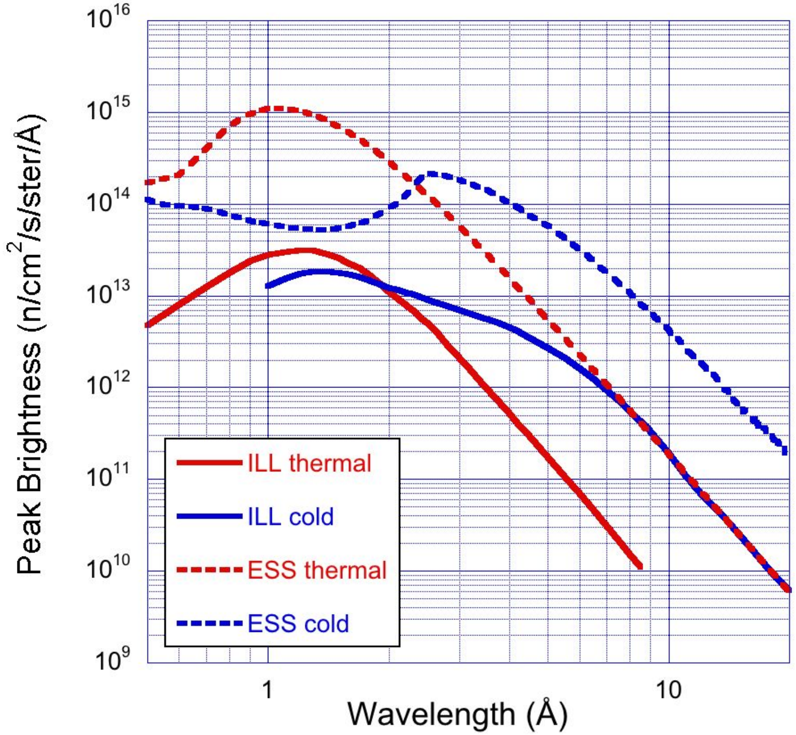
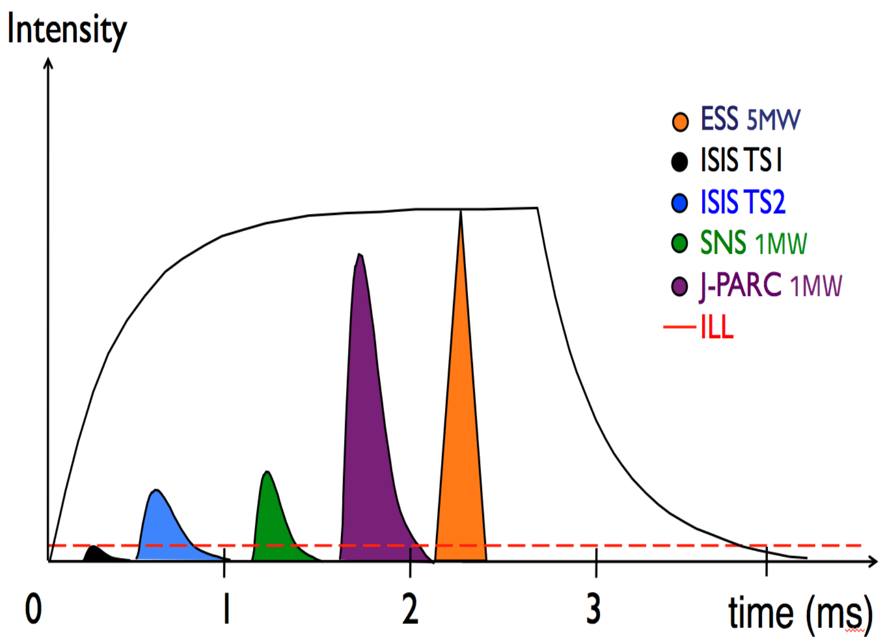
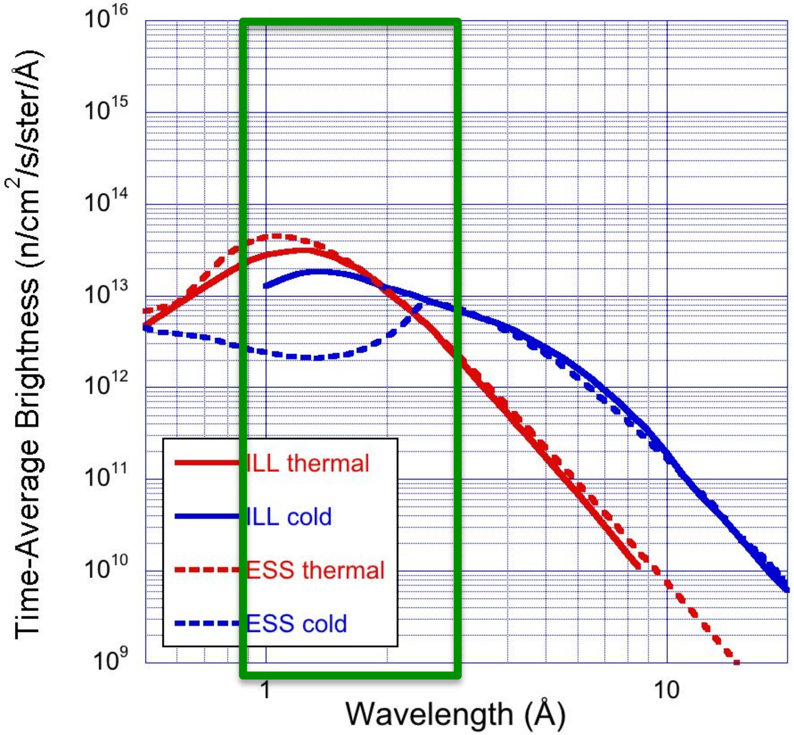
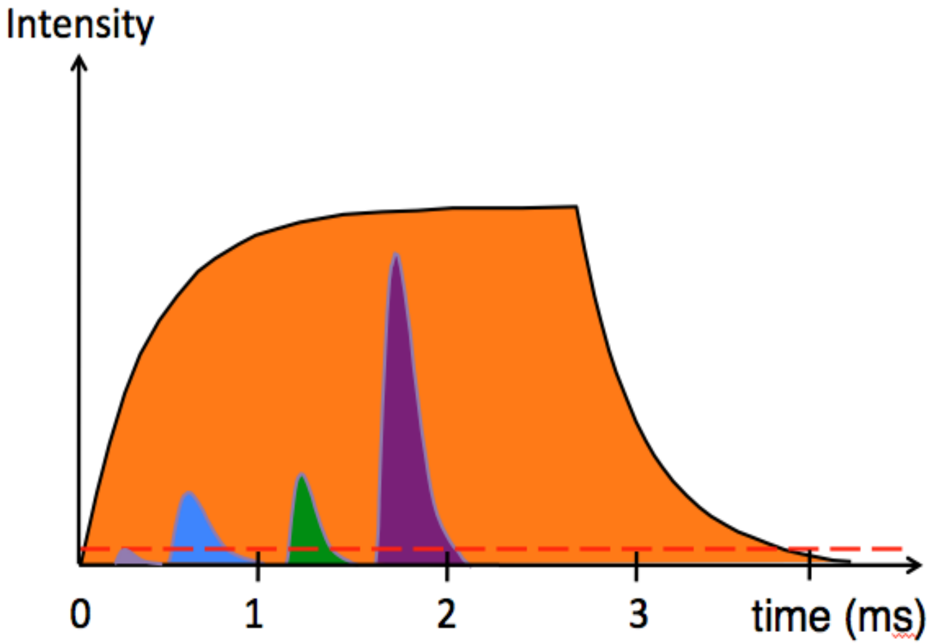
# Why TOF for PD?



# Why Monochromatic for PD?



# Science Drivers for a GPPD

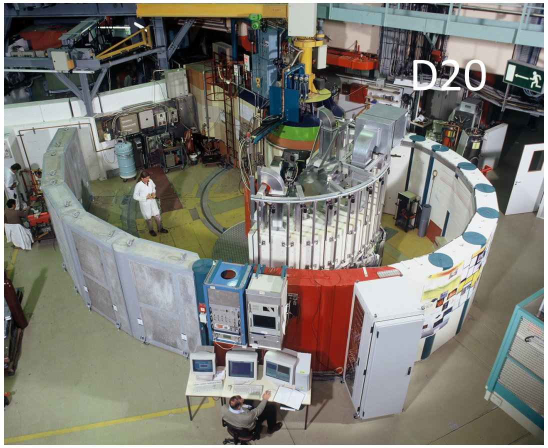
A general purpose powder diffractometer (GPPD) MUST address a wide user community:

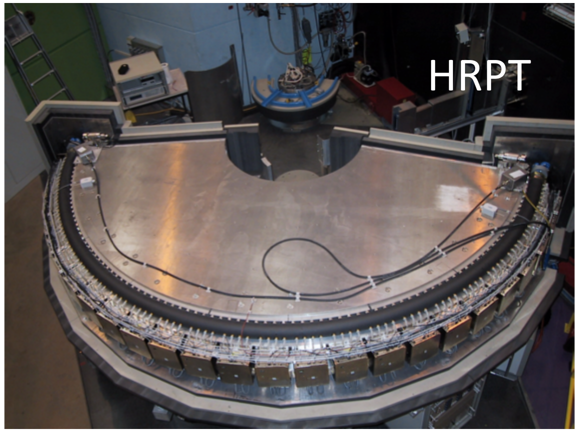
- Nuclear & magnetic structure (crystallography)
  - Small to medium unit cells (< 2000 $Å^3$)
  - Good Q-range coverage ($Q_{max}$ at least 12.0 $Å^{-1}$, preferably 20 $Å^{-1}$)
  - Medium to high resolution ($\Delta d/d$ <1%, preferably approaching 0.1%)
  - Flexible set-up
- *In situ* processing
  - High flux
  - Large detector coverage
  - Large, open sample space
  - Availability of wide range of sample environment
- Additional specialist capabilities?
  - Texture
  - Single crystal
  - Polarisation

# GPPD using monochromators

- Nuclear & magnetic structure (crystallography)
  - Small to medium unit cells (< 2000 Å$^3$) ✔
  - Good Q-range coverage ($Q_{max}$ at least 12.0 Å$^{-1}$, preferably 20 Å$^{-1}$) ✔ 12 Å$^{-1}$
  - Medium to high resolution (Δd/d <1% preferably approaching 0.1%) ✔
  - Flexible set-up ✔
- *In situ* processing
  - High flux ✔
  - Large detector coverage ✔ single side
  - Large, open sample space ✔ side access
  - Availability of wide range of sample environment ✔
- Additional specialist capabilities?
  - Texture — 2D detector
  - Single crystal — 2D detector
  - Polarised beam ✔

# Variable resolution NPDs

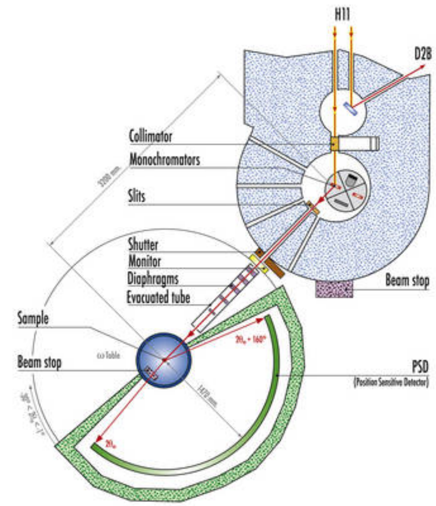



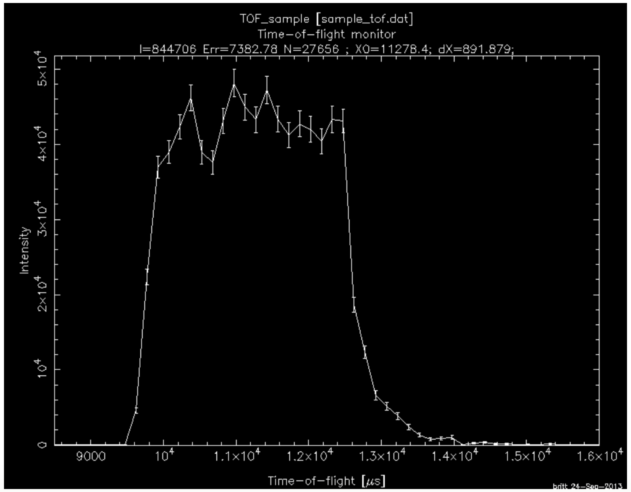




| | WOMBAT-ANSTO | D20 - ILL | HRPT - SINQ |
|---|---|---|---|
| Area detector coverage / ° | 120 | 153.6 | 160 |
| Number of detectors | 960 | 1536 | 1600 |
| Detector angular resolution / ° | 0.125 | 0.1 | 0.1 |
| Sample – detector distance / cm | 70 | 147 | 150 |
| Detector solid angle / Sr | 0.6 | 0.28 | 0.28 |
| Flux for HOPG(002) at 42° takeoff / n $cm^{-2}$ $s^{-1}$ | $1.3 \times 10^{8}$ (est.) | $4.2 \times 10^{7}$ | - |
| Flux for Ge(115) at 120° takeoff / n $cm^{-2}$ $s^{-1}$ | - | $8.0 \times 10^{6}$ | $2.4 \times 10^{5}$ |

# Initial model

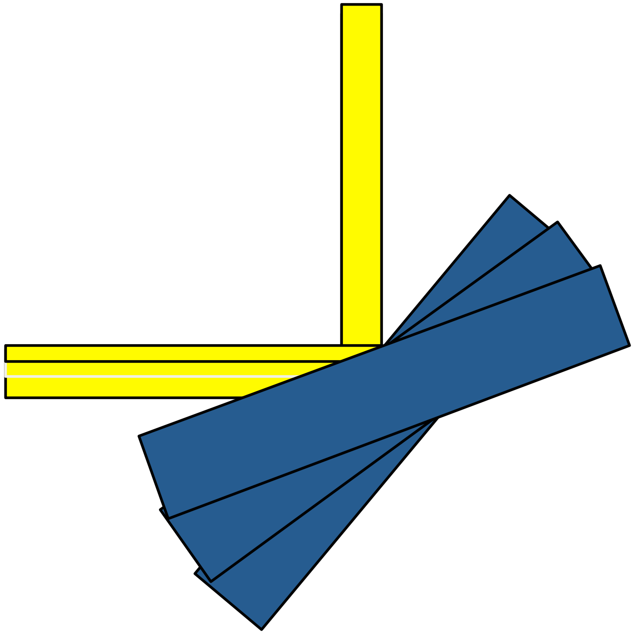
- D20 on the ESS source cf. verified ILL model (based on flux measurements in H11, at sample position and real data)
- D20 uses only 1/3 of beam from H11
- Single λ performance as expected
- Non-optimised model
- Lower backgrounds
- No extra use of TOF capability of the detector

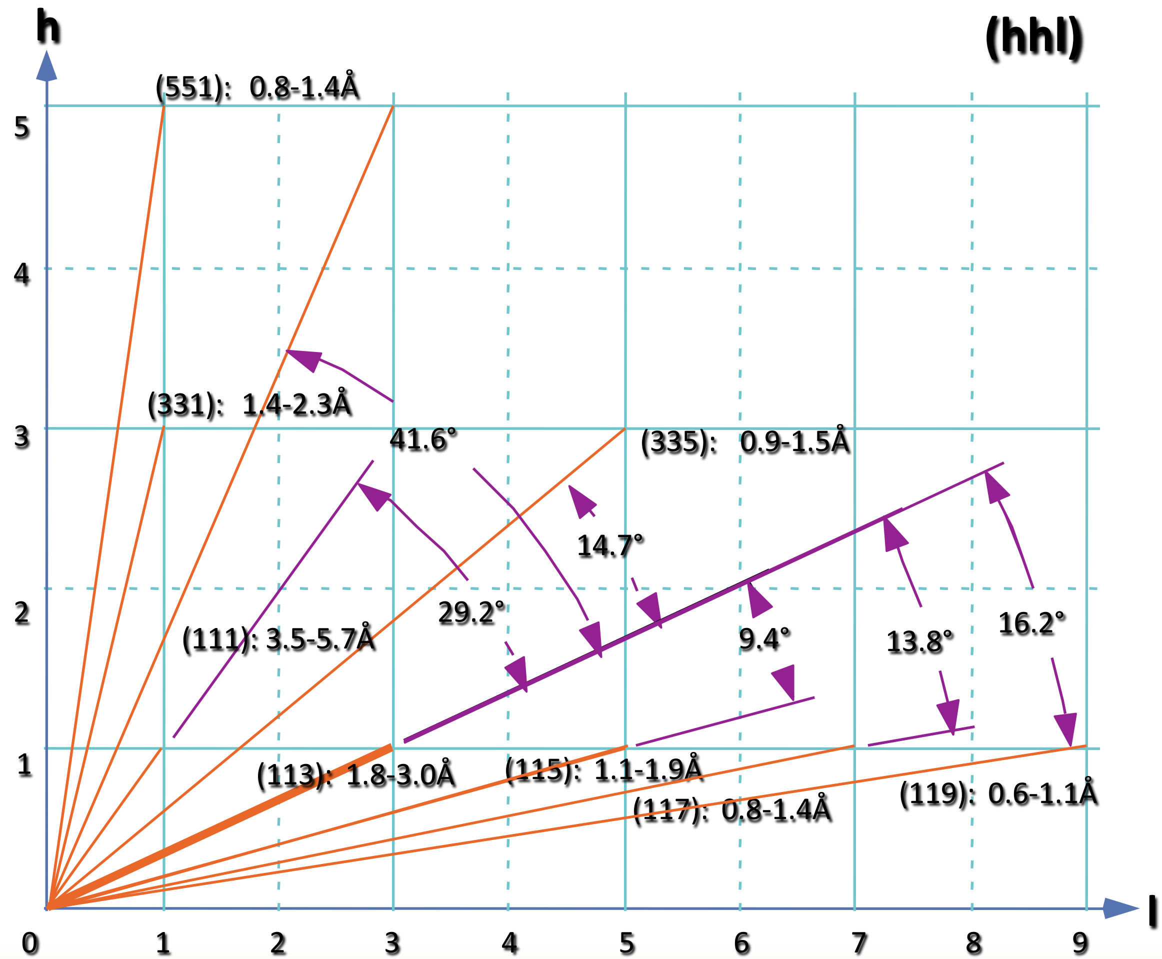


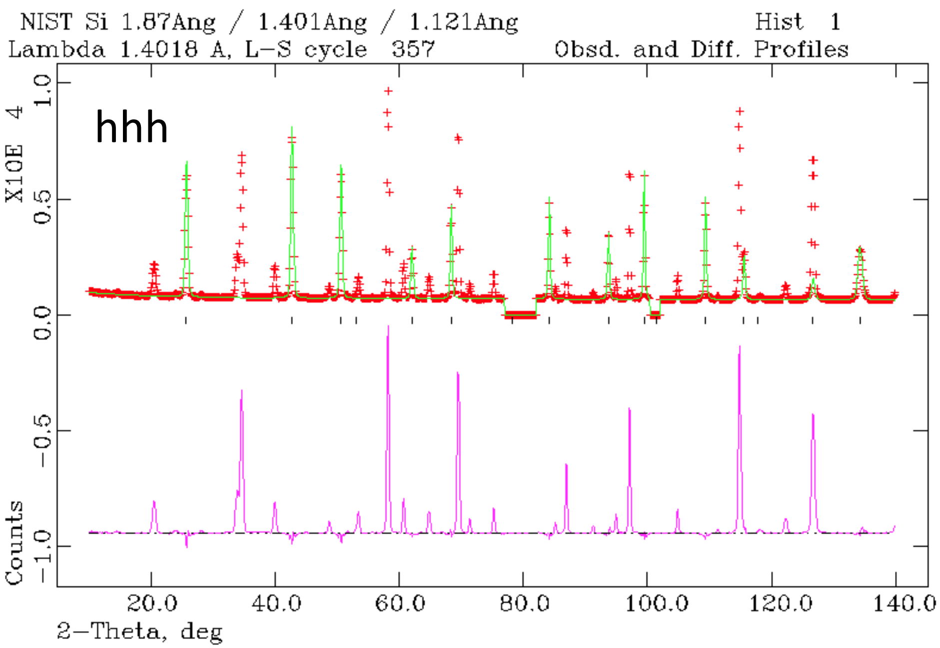

How can we modify the instrument to take advantage of a long pulse source time structure?

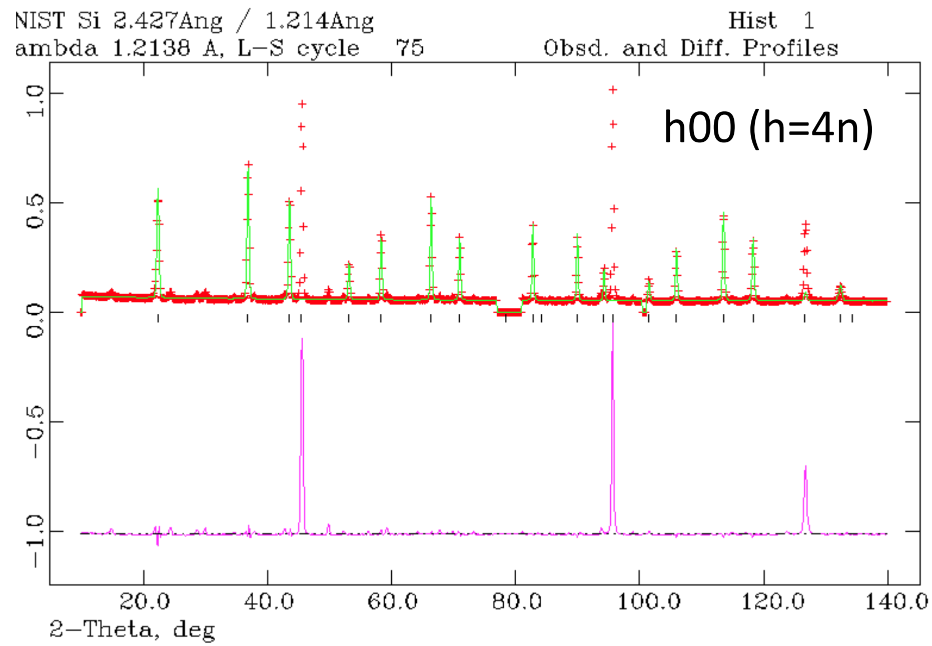
# Multi-wavelength diffraction data?





# Yes! – separate using TOF channel




- Gain in count rate and Q-range
- Resolution minimum for each λ at different Q
- Increase overall instrument length to increase TOF λ separation

# Using TOF to separate λ at detector

For ≈22 m total flight path length (D20) using (h00), 118° takeoff angle:

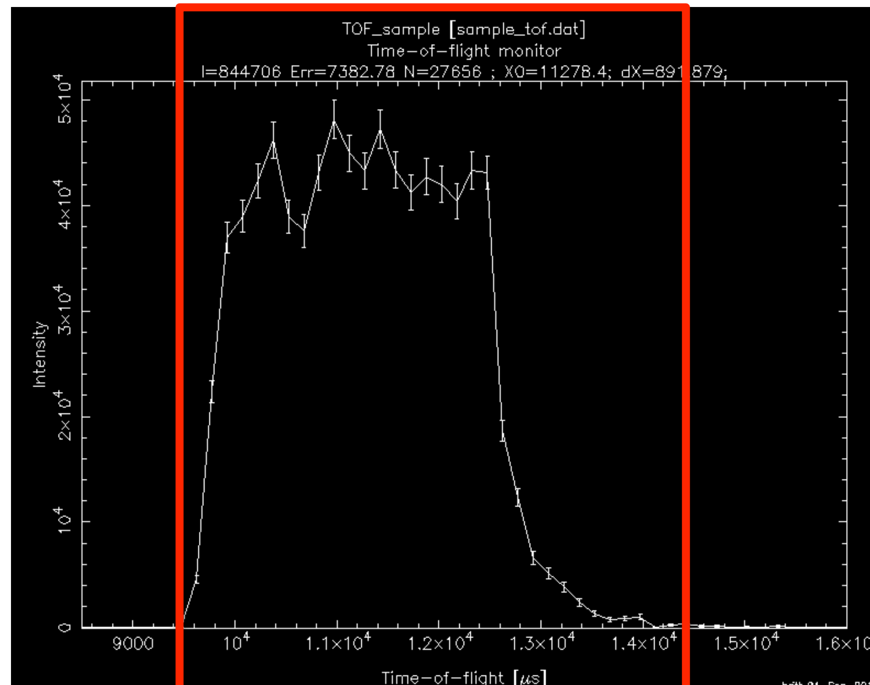
(400) – 2.42 Å take 13.46 ms

(800) – 1.21 Å take 6.73 ms

(1200) – 0.805 Å take 4.477 ms

Wavelength difference required ≈ 0.9 Å

Maximum wavelength in 1st frame 11.5 Å




For 50 m total flight path length:

(400) – 2.42 Å take 30.6 ms

(800) – 1.21 Å take 15.3 ms

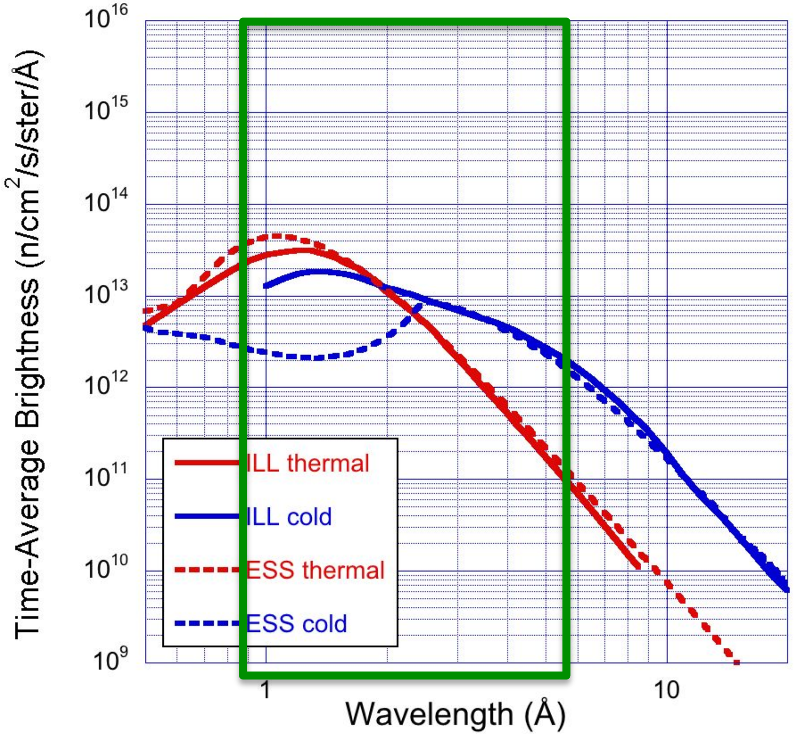
(1200) – 0.805 Å take 10.2 ms

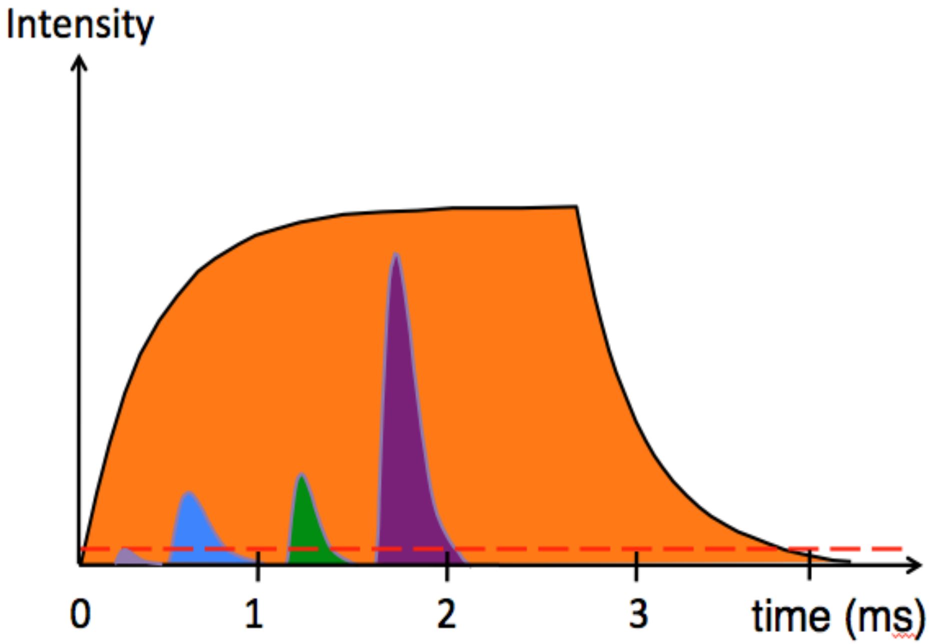
Wavelength difference required ≈ 0.4 Å

Maximum wavelength in 1st frame 5.1 Å

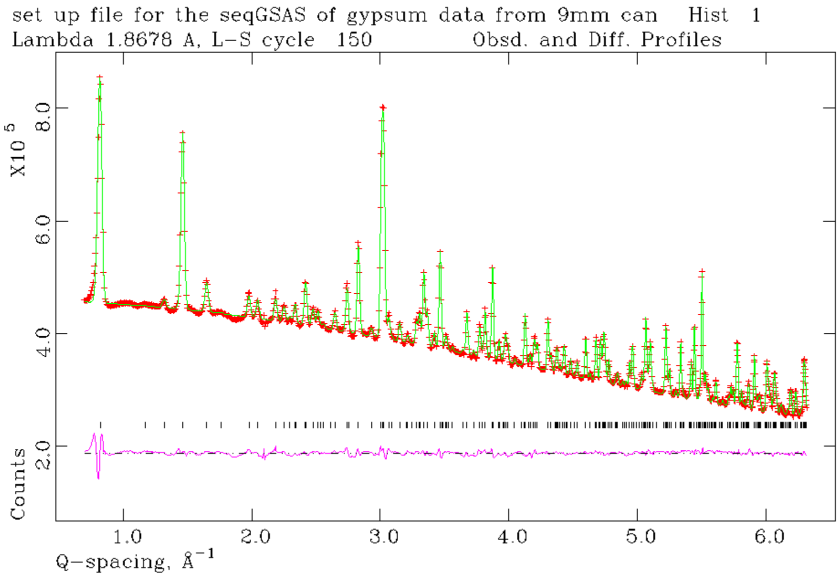
Look to develop monochromator materials with desired properties

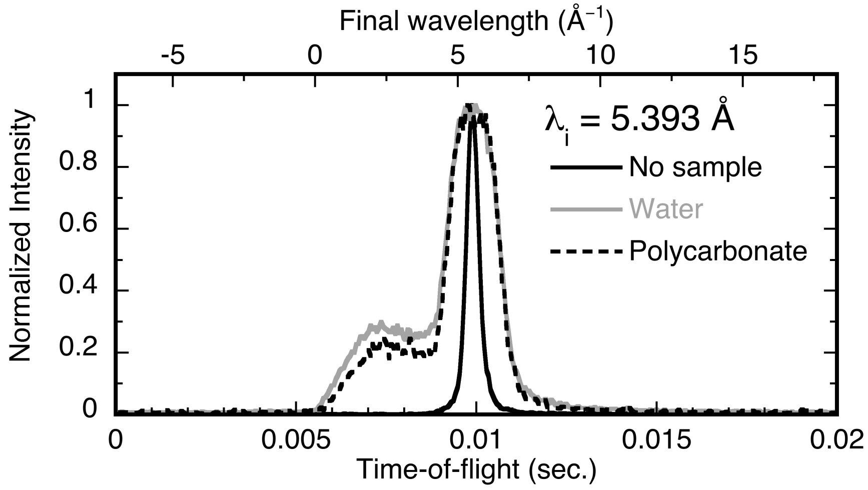
# Extended λ range - bispectral extraction



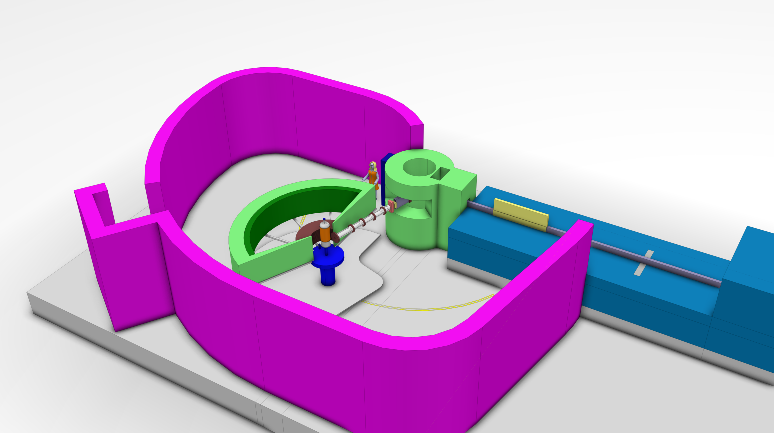



# Incoherent / inelastic scattering



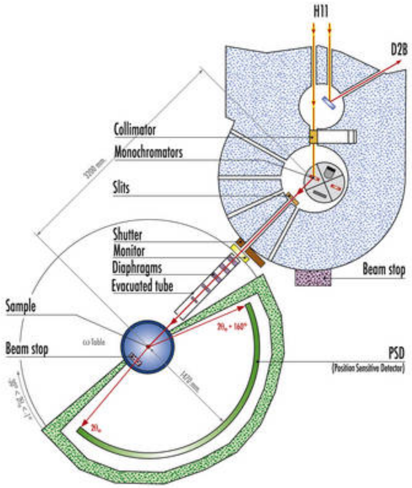



# Current model



Broadly similar to existing reactor instruments
Bispectral extraction
Longer primary flight path – 45m v 17m
Feeder plus half ballistic guide
Continuous takeoff angle
Larger 2D detector – 1 Sr cf. 0.28 Sr

Potential gains
Lower backgrounds (factor 1-1.5)
Multi-wavelength (factor 2-3)
Detector (factor 3.5)




Additional capabilities
TOF channel for energy dispersive measurements
Single crystal + texture measurements

# Summary

- MODI is a flexible GPPD instrument optimised for powder diffraction and *in situ* processing
  - TOF detector channel is used for energy dispersive measurements (elastic or inelastic)
  - 2D detector allows texture and single crystal measurements
- MODI can profit from bispectral extraction to extend useable λ range
- MODI has an open sample space required for the use of complex in situ sample environments
- MODI matches detector coverage (±10°) to restricted geometries available for complex sample environments
- Possibility for diffraction farm
- Need to optimise the thermal moderator performance